LBM 27th Oct 2016 

## 1 Continuum Mechanics.

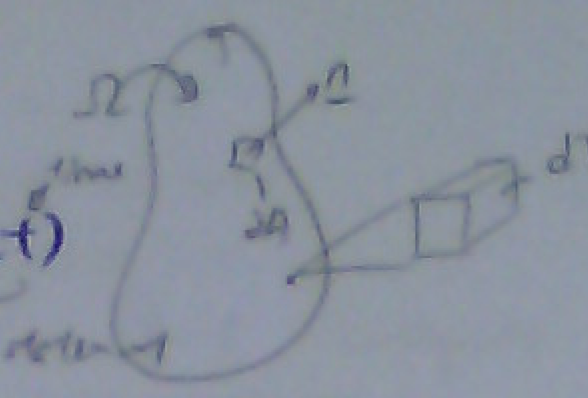
Goal: Derive Navier Stokes equations. in $\mathbb{R}^3$

assume density is apriori defined
such as an average of gas molecules condensed in $dV$

(1.1) Control Volume

w.l.o.g. $\Omega \neq \Omega(t)$

assumed stationary determined



$dV$ $dm = \rho(x)\, dV$

Knudsen number: $\frac{\lambda}{L}$ m.f.p, characteristic length.

Consider Rate of Change of (...)

i. mass.

$$\frac{d}{dt}\int_{\Omega} \rho\, dV = - \int_{\partial\Omega} \rho u \cdot n\, dA \Rightarrow -\frac{d}{dt}\int_{\partial\Omega} \rho u\cdot n\, dA\, dt \qquad (1)$$

$dm = \rho u \cdot n\, dt$

$\underline{u} \cdot n\, dt$

ii. momentum (Newton), $i = 1, 2, 3$ direction, $\underline{u} = (u_1, u_2, u_3)^T$

$$\frac{d}{dt}\int_V \rho u_i\, dV$$

same direction as above, momentum carried away from CV.

$$= - \int_{\partial\Omega} (\rho u_i)\, \underline{u}\cdot\underline{n}\, dA + \int_{\partial\Omega} t_i\, dA \quad ; \quad t_i = \sigma_{ij} n_j \rightarrow \begin{bmatrix} \sigma_{1j} n_j \\ \sigma_{2j} n_j \\ \sigma_{3j} n_j \end{bmatrix} = \sum_{j=1}^{3} \sigma_{ij} n_j$$

summation (einstein notation)

$\underline{\underline{\sigma}} = (\sigma_{ij})_{ij} = 1,2,3$ stress tensor (symm.)

acting against the normal of surface (which points outward)

$$\sigma_{ij} = -\underbrace{p\,\delta_{ij}}_{\substack{\text{diagonal} \\ \text{(principal)}}} + \underbrace{\tau_{ij}}_{\substack{\text{offdiagonal} \\ \text{(shear stress)}}}$$

$$\boxed{\Rightarrow \frac{d}{dt}\int_V \rho u_i\, dV = - \int_{\partial\Omega} \rho u_i\, \underline{u}\cdot\underline{n}\, dA - \int_{\partial\Omega} p\,\underline{n}\, dA + \int_{\partial\Omega} \underline{\underline{\tau}}\, \underline{n}\, dA} \qquad (2)$$

energy done from surface forces

iii. Energy:

energy carried away from CV

$$\frac{d}{dt}\int E\, dV = - \int_{\partial\Omega} E\, \underline{u}\cdot\underline{n}\, dA - \int_{\partial\Omega} p\,\underline{u}\cdot\underline{n}\, dA + \int_{\partial\Omega} (\underline{\underline{\tau}}\, \underline{u})\cdot\underline{n}\, dA - \int_{\partial\Omega} \underset{\text{heat.}}{q}\cdot\underline{n}\, dA \qquad (3)$$

**Use Divergence Theorem:**

(i) $\int_{\Omega} \frac{d}{dt}\rho\, dV + \int_{\Omega} \nabla\cdot(\rho\underline{u})\, dV = 0$ $\qquad \frac{d}{dt}\rho + \nabla\cdot(\rho\underline{u}) = 0$

(ii) $\int_{\Omega} \left( \frac{\partial \rho u}{\partial t} + \nabla\cdot(\rho\, \underline{u}\otimes\underline{u}) + \nabla p - \nabla\cdot\underline{\underline{\tau}} \right) dV = 0$ ; $\underline{u}\otimes\underline{u} = (u_i u_j)$ $i,j = 1,2,3$

(iii) $\int_{\Omega} \left( \frac{\partial E}{\partial t} + \nabla\cdot(E\underline{u}) + \nabla\cdot(p\underline{u}) - \nabla\cdot(\underline{\underline{\tau}}\,\underline{u}) + \nabla\cdot q \right) dV = 0$

can't solve the three pdes, as there are 15 unknowns but 5 eqn.

$\rho, u_1, u_2, u_3, E$

$\tau \Rightarrow 6$, $\underline{u} \Rightarrow 3$, $q \Rightarrow 3$, $p = 1$

To close the system:

(1.2) Equation of state:

$$P = \rho R T \quad , R \text{ - specific gas constant.}$$

$$R = c_p - c_v \quad \text{heat capacity at constant } p \text{ \& } v$$

$$= c_v\left(\frac{c_p}{c_v} - 1\right) \quad ; \quad \gamma = \frac{c_p}{c_v}$$

$$\Rightarrow RT = (\gamma - 1)\, c_v T$$

$c_v T$: $e_{int}$ (specific int. energy), "calorically perfect gas" } allowed by ideal gas assumption

Now:

energy per unit volume

$$E = \rho e_{int} + \frac{1}{2}\rho \|u\|^2$$

internal energy, kin. energy

$$\Rightarrow \rho e_{int} = E - \frac{1}{2}\rho\|u\|^2$$

by ideal gas law:

$$P = \rho\underbrace{(\gamma-1)c_v T}_{RT} = \rho(\gamma-1)e_{int} = (\gamma-1)\left(E - \frac{1}{2}\rho\|u\|^2\right)$$

, hence we reduced an unknown 'P'

$$P = \rho R T \quad ; \quad R = \frac{J}{kg \cdot K} = \frac{\hat{R}}{M}$$

$\hat{R}$: universal gas constant; $M$: molar weight. $[M] = \frac{kg}{mol}$ (mass of 1 mol)

$$P = \rho \frac{\hat{R}}{M} T \quad ; \quad M = m \cdot N_A$$

$N_A$: avogadro's constant; $m$: mass of one molecule.

$$= \frac{\rho}{m}\frac{\hat{R}}{N_A} T$$

$\frac{\rho}{m}$: $n$ number density; $\frac{\hat{R}}{N_A}$: $k_b$ Boltzmann constant

Finally: $\rho = n k_B T$ in this representation, it doesn't matter which species of gas is depicted. What matters is just the number of molecules in the gas

(1.3) ~~Consecutive laws.~~ Constitutive Laws.

(i) Newtonian Fluids.

$$\tau_{ij} = C_{ijkl}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right)$$

$C_{ijkl}$: 4th order tensor

We want:

- homogeneity
- isotropy.

$$\Rightarrow C_{ijkl} = \lambda \delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

$$\Rightarrow \tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \lambda\frac{\partial u_k}{\partial x_k}$$

As a result, $\tau$ depends only on $\underline{u}$ & $\underline{x}$!

often: $\lambda = -\frac{2}{3}\mu$ "Stokes Hypothesis"

chosen such that $\tau_j$ is traceless, $\tau_{ii} = 0$, should we then after substituting, the principal stresses are not affected.

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(ii) Fourier's Law

$$\underline{q} = -k\nabla T$$ from $RT = (\gamma-1)(E - \frac{1}{2}\rho\|u\|^2)$

coefficient of heat conduction

hence, we reduced another unknown $\underline{q}$

~~Inc~~ Incompressible N-S

$$\nabla \cdot \underline{u} = 0$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0}\frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} \; ; \; \nu = \frac{\mu}{\rho_0}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{u}) = 0 \; ; \quad \nabla = \frac{\partial^2}{\partial x_j \partial x_j}$$

LBM 27th Oct 2016 (tutorial)

Intro to Probability Theory

(1) Sample space and Probability.

(1.1) $\Omega := \{$"All possible outcomes of an Experiment"$\}$

Example

(E1) $\Omega := \{1, 2, 3, 4, 5, 6\}$ to roll a die

(E2) $\Omega := \{$"heads", "tails"$\}$ to flip a coin.

(E3) $\Omega := \{1, 2, 3, \ldots\} \equiv \mathbb{N}$ How many time will we get red? (in roulette)

For now: finite or countably infinite sample space

(1.2) Events $A \subset \Omega$

Example: (E1) "Even number" $A = \{2, 4, 6\} \subset \Omega$

Elementary event: Singleton set containing only one element $w \in \Omega$ $A = \{w\}$

(1.3) Probability : $P : \mathcal{P}(\Omega) \to [0,1]$

$\uparrow$ power set, set of all sets

probability of everything or any events

s.th : $P(\Omega) = 1$

finite $\Omega$ : $P(A_1) + P(A_2) = P(A_1 \cup A_2)$, $A_1 \cap A_2 = \emptyset$

infinite $\Omega$ : $\sum_{n=1}^{\infty} P(A_i) = P(\bigcup_{n=1}^{\infty} A_n)$

($\sigma$ - additivity)

We call $(\Omega, P)$ a probability space.

Example:

E1 "Even number" $A_1 = \{2, 4, 6\}$

"Odd number" $A_2 = \{1, 3, 5\}$

If we assume ~~$P(\{w_i\}) = \frac{1}{6}$~~ ~~$i = 1, \dots, 6$~~ $P(\{w_i\}) = \frac{1}{6}$, $i = 1, \dots, 6$

Then $P(A_1) = \frac{1}{2} = P(A_2)$

$P(A_1) + P(A_2) = 1 = P(A_1 \cup A_2)$

Probability Function

$P(\{w_i\}) = p(w_i)$

$\rightarrow 1 = \sum_{w \in \Omega} p(w)$

"probability of elementary events"

Example: AKA (Laplace model $p(w) = \frac{1}{\#\Omega}$, $P(A) = \frac{\#A}{\#\Omega}$)

E1 $p(w) = \frac{1}{6}$ $\forall w \in \Omega$

E2 $p(w) = \frac{1}{2}$ $\forall w \in \Omega$

E3 $p(1) = \frac{18}{37}$ ← # red balls / ← all balls

$p(2) = \frac{19}{37} \cdot \frac{18}{37}$

$p(3) = \left(\frac{19}{37}\right)^2 \cdot \frac{18}{37}$

$p(n) = \left(\frac{19}{37}\right)^{n-1} \cdot \frac{18}{37}$

(1.3) Probability : $P : \mathcal{P}(\Omega) \to [0,1]$

power set: set of all sets

probability of everything = [illegible]

s.th. : $P(\Omega) = 1$

finite $\Omega$ : $P(A_1) + P(A_2) = P(A_1 \cup A_2)$, $A_1 \cap A_2 = \emptyset$

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We call $(\Omega, P)$ a probability space.

Example:

(E1) "Even number" $A_1 = \{2, 4, 6\}$

"Odd number" $A_2 = \{1, 3, 5\}$

If we choose ~~$P(\{\omega_i\}) = \frac{1}{6}$~~ ~~$i = 1, \dots, 6$~~ $P(\{\omega_i\}) = \frac{1}{6}$, $i = 1, \dots, 6$

Then $P(A_1) = \frac{1}{2} = P(A_2)$

$P(A_1) + P(A_2) = 1 = P(A_1 \cup A_2)$

Probability Function

$P(\{\omega_i\}) = p(\omega_i)$

$\to 1 = \sum_{\omega \in \Omega} p(\omega)$

"probability of elementary events"

Example: AKA (Laplace model) $p(\omega) = \frac{1}{\#\Omega}$, $P(A) = \frac{\#A}{\#\Omega}$)

(E1) $p(\omega) = \frac{1}{6}$ $\forall \omega \in \Omega$

(E2) $p(\omega) = \frac{1}{2}$ $\forall \omega \in \Omega$

(E3) $p(1) = \frac{18}{37}$ (# red bins / # all bins)

$p(2) = \frac{19}{37} \cdot \frac{18}{37}$

$p(3) = \left(\frac{19}{37}\right)^2 \cdot \frac{18}{37}$

⋮

$p(n) = \left(\frac{19}{37}\right)^{n-1} \cdot \frac{18}{37}$

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Check:

$$\sum_{n=1}^{\infty} p(n) = \frac{18}{37} \sum_{r=0}^{\infty} \Big(\underbrace{\frac{19}{37}}_{q<1}\Big)^r$$

geometric series

$$= \frac{18}{37} \cdot \frac{1}{1-q}$$

$$= 1.$$

(1.4) Multivariate Probability

$$\Omega^n = \Omega \times \Omega \times \Omega \ldots \times \Omega := \{(a_1, \ldots, a_n) : a_i \in \Omega\}$$

Example "Two dice"

E1

$$\Omega^2 = \Omega \times \Omega := \{(a_1, a_2) : a_i \in \Omega\}$$

$$w_i \in \Omega^2 = (a_1, a_2) \quad a_i \in \{1, 2, 3, 4, 5, 6\}$$

$$p(w_i) = \frac{1}{36}$$

② Random variables

$$X : \Omega \to \mathbb{R}$$

$$p(X = a) = p(a) = \sum_{\substack{w \in \Omega \\ X(w) = a}} p(w)$$

function that takes elementary events (w) as input, that gives new events.

Example: E1 "two dice"

$$w = (i, j) \quad i, j = 1, \ldots, 6$$

$$X(w) = i + j$$

$$\{w \in \Omega : X(w) = 5\} = \{X = 5\} = \{(1,4), (4,1), (3,2), (2,3)\}$$

$$P(X = 5) = \frac{4}{36} = \frac{1}{9}.$$

(E2) $\{$"heads", "tails"$\}$

$X(\text{"heads"}) = +1$

$X(\text{"tails"}) = -1$

(E1) $X(w) = \begin{cases} -2000 & w = \{1,2,3,4\} \\ +5000 & w = \{5,6\} \end{cases}$ ← would you play?

(any die)

## (3) moments

### (3.1) Expectation values

~~expected~~ outcome of event

$$\mu(X) = \sum_{w \in \Omega} X(w)\, p(w)$$

expectation value function

probability of the event

Consider above (E1),

$$\mu(X) = \sum_{w \in \Omega} -2000 \cdot \frac{2}{3} + 5000 \cdot \frac{1}{3} \approx +333$$

### (3.2) $\mu(F(x)) = \sum_{w \in \Omega} F(X(w))\, p(w)$

e.g. $\mu(X^k) = \sum_{w \in \Omega} X^k p(w)$

**Example:** variance, outcome, expected outcome

$$\sigma^2(X) = \mu\left((X - \mu(X))^2\right)$$

not linear !!!

$$= \mu\left(X^2 - 2X\mu(X) + \mu(X)^2\right)$$ apply $\mu$ function to each of the terms.

$$= \mu(X^2) - 2\mu(X)\mu(X) + \mu(X)^2$$ expectation value of a constant, is the constant itself.

$$= \mu(X^2) - \mu(X)^2$$

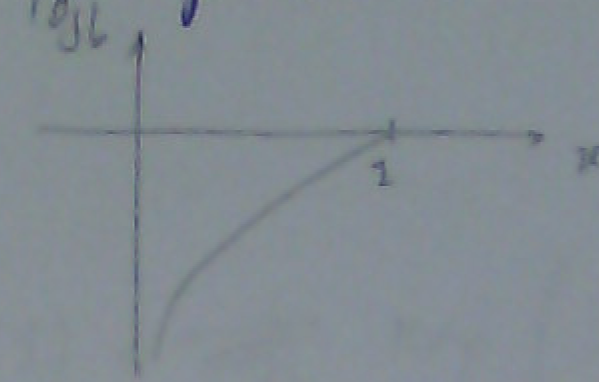
### (3.3) standardised distribution

$$X \mapsto X^* = \frac{X - \mu(X)}{\sigma(X)} \Rightarrow \mu(X) = 0$$

## 4 Information Entropy

(4.1) "Self - Information" or "Surprise"

$$I(\omega) = \underbrace{-\log_b(p(\omega))}_{\text{negative}} \geq 0$$




Example:

$p(\omega) = 1 \Rightarrow I(\omega) = 0$

$p(\omega) \to 0 \Rightarrow I(\omega) \to \infty$

Let $b = 2$, for event E2

$\Omega := \{\text{"heads"}, \text{"tails"}\}$

$p(\omega) = \frac{1}{2}$

$I(\omega) = 1$

(4.2) Information Entropy $\rightarrow$ $H = \mu(I) = -\sum_{\omega \in \Omega} p(\omega) \log(p(\omega))$

E2 $\Omega := \{\text{"heads"}, \text{"tails"}\}$

(i) "Fair coin" $p(\omega) = \frac{1}{2}$

$H = 1 \quad \left( -\sum_{\omega \in \Omega} \frac{1}{2}(-1) \right)$

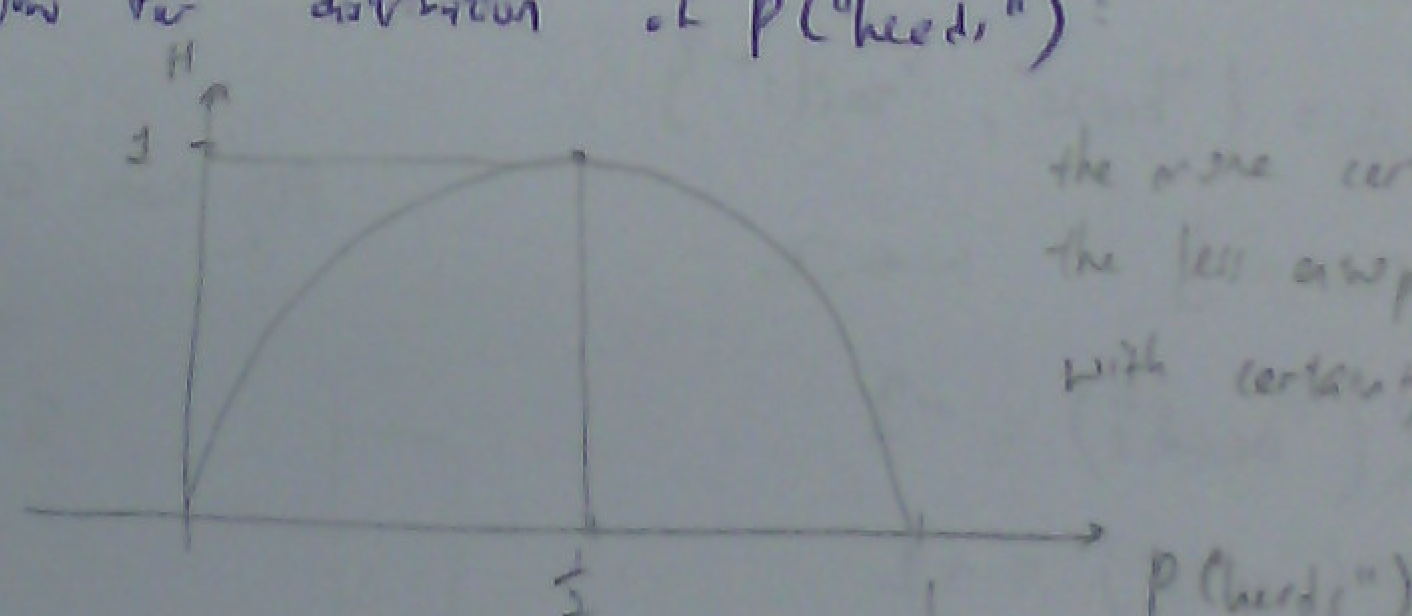
(ii) "unfair coin"

$p(\text{"heads"}) = 1$

$p(\text{"tails"}) = 0$

$H = 0$

Now for distribution of $P(\text{"heads"})$:




the more certain of the outcome, the less entropy it has. with certainty, $H \to 0$

## 5 Continuous Sample Space

(5.1) probability density function.

$f : \mathbb{R} \to [0, \infty)$

$\int_{\mathbb{R}} f \, dx = 1$

$P(a \leq X \leq b) = \int_a^b f \, dx$

Example: Gaussian distribution

$$f(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(\frac{-(x-\mu)^2}{\sigma^2}\right) =: N(\mu, \sigma)$$

multivariate case:

$$f : \mathbb{R}^n \to [0, \infty)$$

$$\underline{x} = (x_1, \dots, x_n)$$

$$\int_{\mathbb{R}^n} f \, dx_1 \dots dx_n = 1$$

(5.2) $$\mu(x) = \int_{\mathbb{R}} x \, f(x) \, dx$$

multivariate case:

$$\mu(x_k) = \int_{\mathbb{R}} x_k \, f(\underline{x}) \underbrace{dx_1 \dots dx_n}_{d\underline{x}}$$

(5.3) Entropy

$$H(f) = -\int_{\mathbb{R}^n} f \ln(f) \, d\underline{x}$$ — H theorem

## ⑥ Central limit theorem

Consider (E2) $\Omega = \{\text{"heads"}, \text{"tails"}\}$

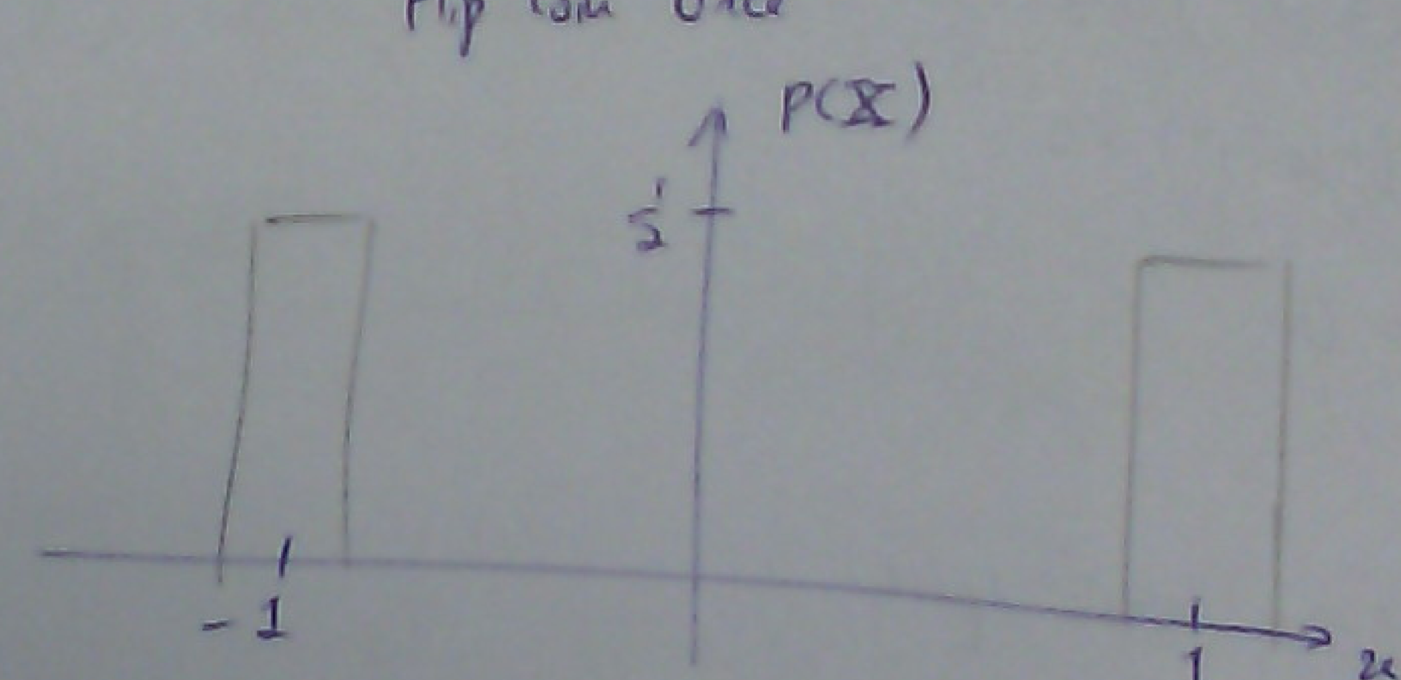
$p(\omega) = \frac{1}{2} \quad \omega \in \Omega$

$X(\text{"heads"}) = -1$

$X(\text{"tails"}) = +1$

$\mu(X) = 0$ rule (5.1)

Flip coin once




Flip twice:

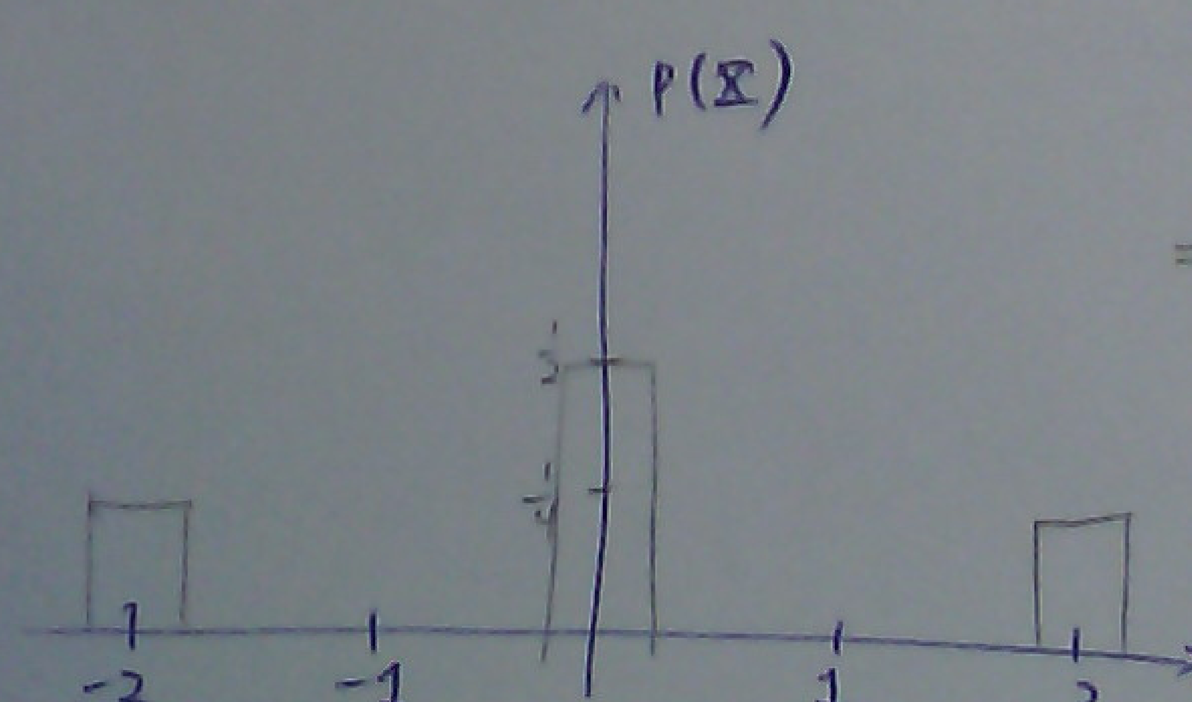
$\Omega^2 = \Omega \times \Omega$

$:= \{(a_1, a_2) : a_i \in \Omega\}$

$X(a_1) = X_1$

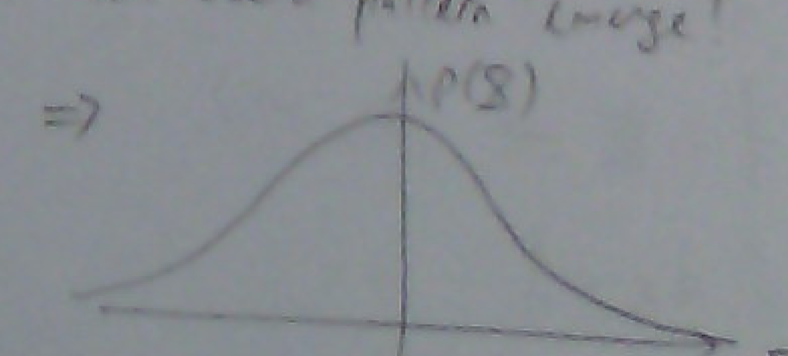
$X(a_2) = X_2$

$X = X_1 + X_2$




$X = X_1 + X_2$

as number of flips increases, we see a pattern emerge!



same laplacian model each time experiment is done



Let $X_1, \dots, X_n$ be independent, identically distributed (iid) random variables

$$a_n = S_n = X_1 + \dots + X_n$$

$$\lim_{n\to\infty} \left( \frac{S_n - \mu(S_n)}{\sigma(S_n)} \right) = N(0,1) = \frac{1}{\sqrt{2\pi}} \exp\left( \frac{-x^2}{2} \right)$$

doesn't have to be laplacian model, as long as model stays the same and independent to each other.

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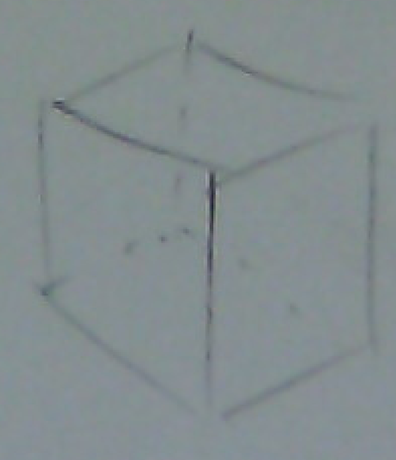
( Ch. 4. The Maxwell-Boltzmann Distribution

We assume:

- binary interactions.
- Spherically symmetric potentials. } not restrictions, but for convenience

$$F = -\phi'(r)$$

force, potential, distance



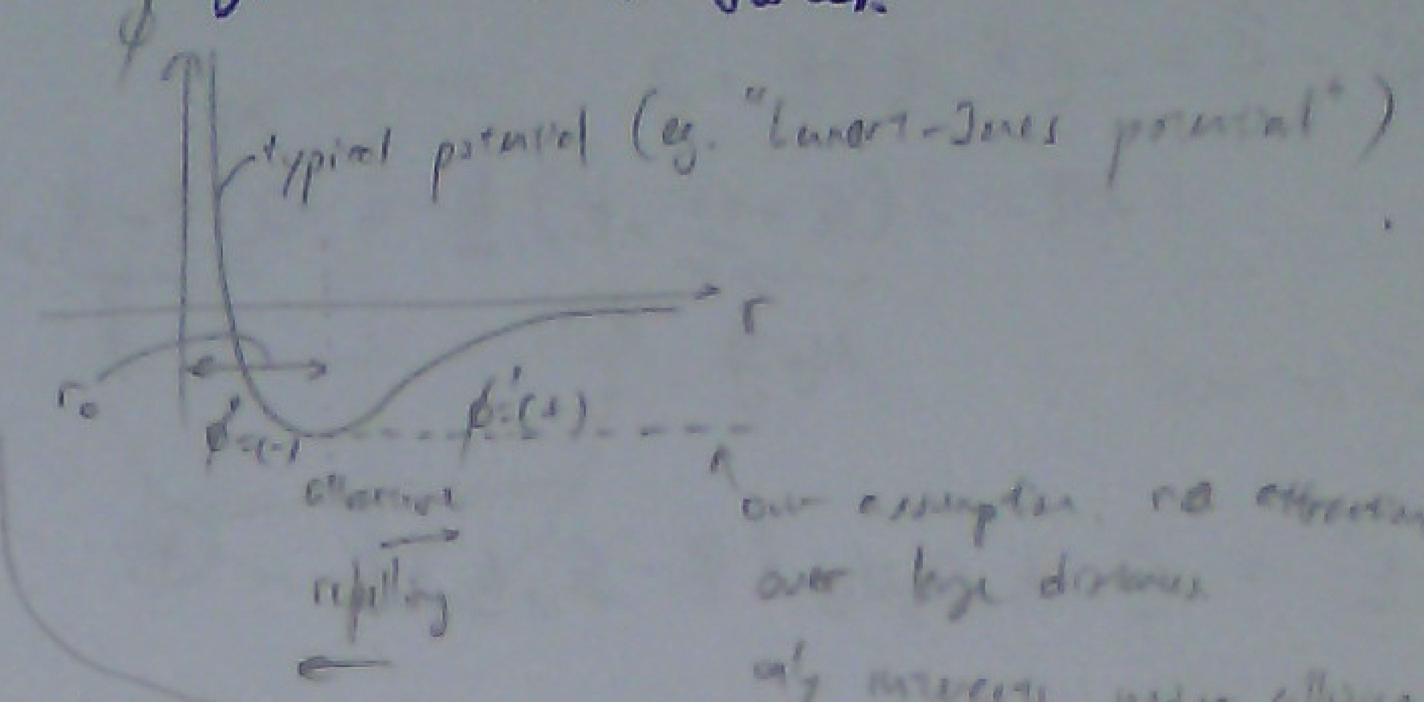
"gas in a box"

$\rho = \rho_0 = \text{const.}$

$T = T_0 = \text{const.}$

etc.

neglected external forces.




## (4.1) Intermolecular interactions

Consider two particles

$m_A, \underline{c}$ @ $t=0$ $\underline{x}_A$ - location $\quad \underline{c} = \dot{\underline{x}}_A$

$m_B, \underline{z}$ $\quad \underline{x}_B$

velocity

$$\underline{x}_m = \frac{\underline{x}_A m_A + \underline{x}_B m_B}{m_A + m_B}$$

"centre of mass"

$$\Rightarrow \underline{w} = \dot{\underline{x}} = \frac{\dot{\underline{x}}_A m_A + \dot{\underline{x}}_B m_B}{m_A + m_B}$$

$$= \frac{\underline{c} m_A + \underline{z} m_B}{m_A + m_B}$$

Note: const velocity ($\underline{w} = \text{const.}$)

Consider reference frame moving with velocity $\underline{w}$

$\hat{\underline{c}} := \underline{c} - \underline{w} = -\mu_B \underline{g}$ (1); $\quad \underline{g} = \underline{z} - \underline{c}$

$\hat{\underline{z}} := \underline{z} - \underline{w} = \mu_A \underline{g}$ (2)

$$\mu_i = \frac{m_i}{m_A + m_B} \quad i = A, B$$

$m_A \hat{\underline{c}}(t) = - m_B \hat{\underline{z}}(t)$

(1),(2)

$\Rightarrow m_A \|\underline{c}\| = m_B \|\underline{z}\| \quad \forall (t)$

Relation between

$\hat{\underline{c}}, \hat{\underline{z}}$ and $\hat{\underline{c}}', \hat{\underline{z}}'$

before, after

Let $\hat{c} = \|\hat{\underline{c}}\|$

$\hat{z} = \|\hat{\underline{z}}\|$

we have:

$m_A \hat{c} = m_B \hat{z}$

$m_A \hat{c}' = m_B \hat{z}'$

$\Rightarrow m_A(\hat{c} + \hat{c}') = m_B(\hat{z} + \hat{z}')$ (3)

$m_A(\hat{c} - \hat{c}') = m_B(\hat{z} - \hat{z}')$ (4)

Kinetic Energy:

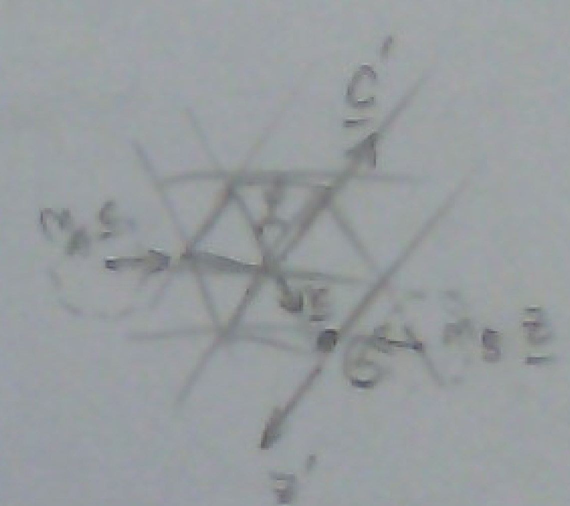
$$\frac{1}{2} m_A \hat{c}^2 + \frac{1}{2} m_B \hat{z}^2 = \frac{1}{2} m_A (\hat{c}')^2 + \frac{1}{2} m_B (\hat{z}')^2$$

Note:

$m_A = m_B \Rightarrow \hat{c} = \hat{c}'$, $\hat{z} = \hat{z}'$

let $m_A \neq m_B$, see notes.

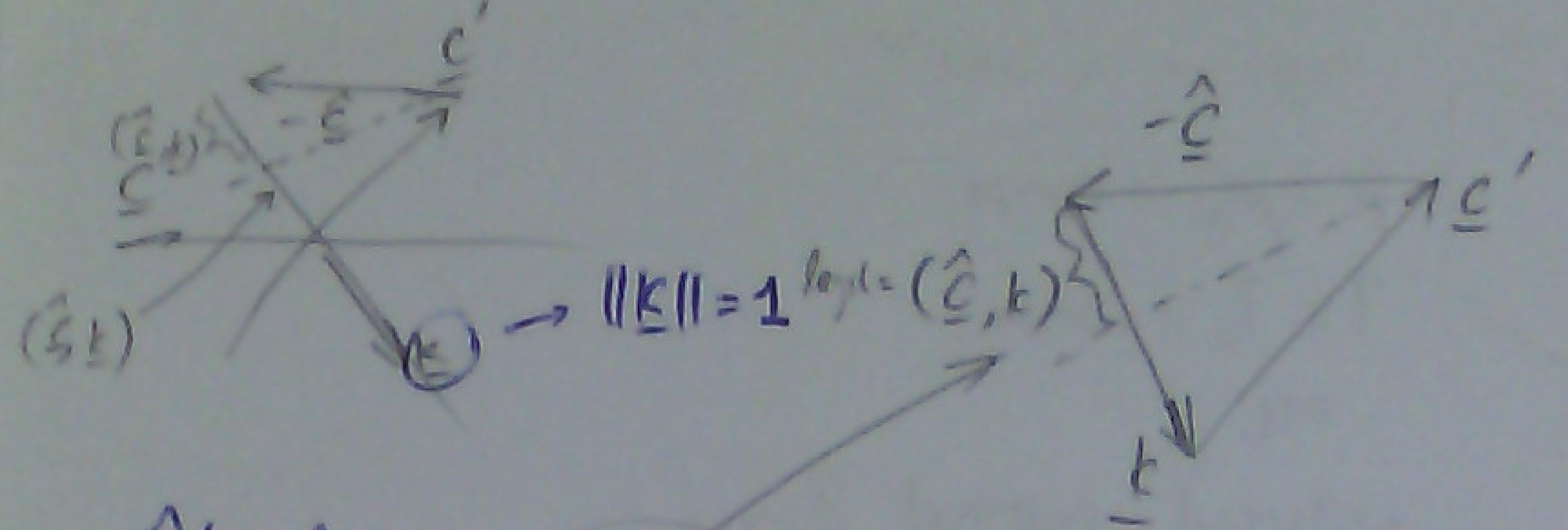
again, we have $\hat{c} = \hat{c}'$, $\hat{z} = \hat{z}'$




Conservation of angular momentum:

$b = b'$ (see figure, take moment about (B))

also: planar motion.




$$\hat{\underline{c}}' - \hat{\underline{c}} = -(\hat{\underline{c}},\underline{k})\,\underline{k}\cdot 2$$

$$= \cancel{A} - 2(\underbrace{\underline{c}-\underline{w}}_{\mu_B\,\underline{g}},\underline{k})\,\underline{k} \quad \text{by (1)} \quad = +2\,\overset{\mu_B}{\wedge}(\underbrace{\underline{z}-\underline{c}}_{\underline{g}},\underline{k})\,\underline{k}$$

note! no hat!

$$\underline{c}' = \underline{c} + 2\mu_B(\underline{z}-\underline{c},\underline{k})\,\underline{k} \quad (*)$$

$$\underline{z}' = \underline{z} - 2\mu_A(\underline{z}-\underline{c},\underline{k})\,\underline{k} \quad (**)$$

$$\begin{pmatrix}\underline{c}'\\ \underline{z}'\end{pmatrix} = \underline{F}(\underline{c},\underline{z}) = \begin{pmatrix}\underline{F}_1(\underline{c},\underline{z})\\ \underline{F}_2(\underline{c},\underline{z})\end{pmatrix}\begin{matrix}(*)\\(**)\end{matrix}$$

Jacobian:

3×3 matrix

$$F' = \left(\begin{array}{c|c} \dfrac{\partial \underline{F}_1}{\partial \underline{c}} & \dfrac{\partial \underline{F}_1}{\partial \underline{z}} \\ \hline \dfrac{\partial \underline{F}_2}{\partial \underline{c}} & \dfrac{\partial \underline{F}_2}{\partial \underline{z}} \end{array}\right)$$

$\det F' = 1$

# LBM 3rd Oct 2016 tutorial

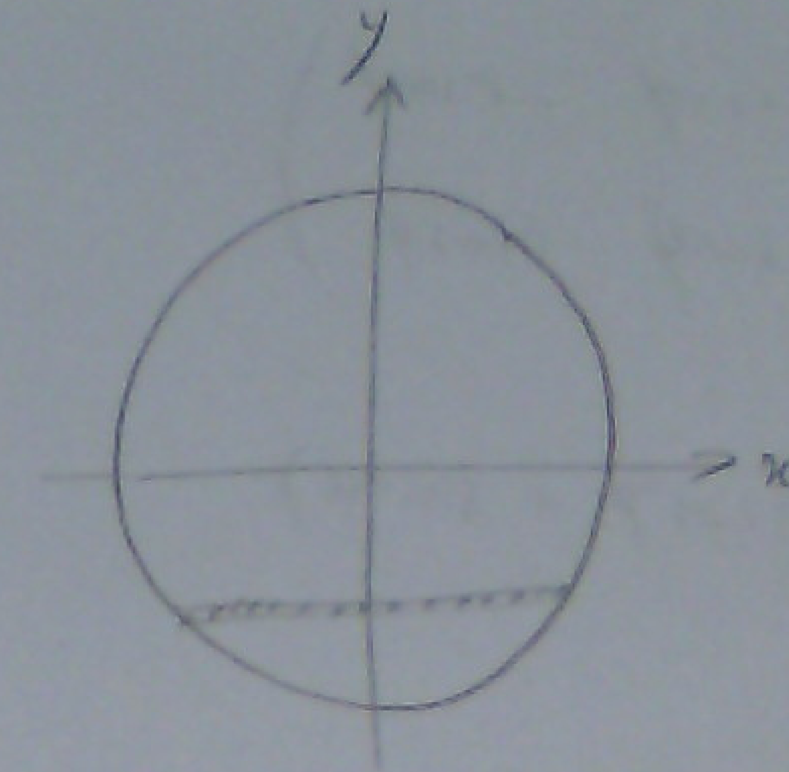
## 1 Integral Transformation

Motivation:

Let $D := \{(x,y) : x^2+y^2 \leq R^2 ; R>0\}$ (*)

Consider:

$$\iint_D f(x,y)\, dx\, dy = \int_{-R}^{R} \int_{-\sqrt{R^2-y^2}}^{\sqrt{R^2-y^2}} f(x,y)\, dx\, dy$$




Let $\Phi : S \longrightarrow D$ be a coordinate transformation.

$(u,v) \longmapsto \Phi(u,v) = (x,y)$

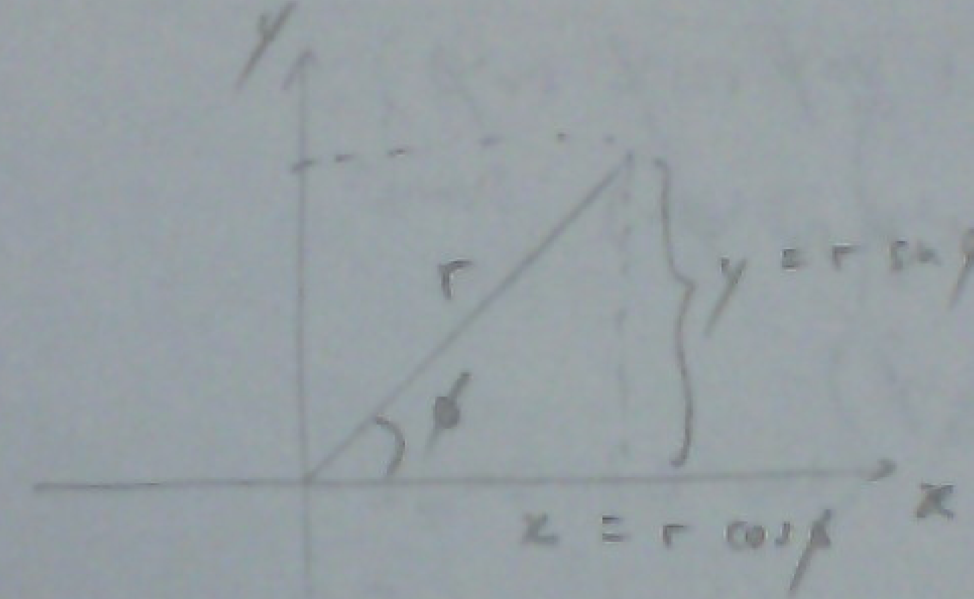
$(u,v,w) \longmapsto \Phi(u,v,w) = (x,y,z)$

**Example** (a) polar coordinates

$u = r$

$v = \phi$

$$\Phi = \begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix}$$




$x = r\cos\phi$

$y = r\sin\phi$

$$\begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \phi} \end{bmatrix} \begin{pmatrix} dr \\ d\phi \end{pmatrix}$$

$$\begin{bmatrix} \cos\phi & -r\sin\phi \\ \sin\phi & r\cos\phi \end{bmatrix}$$

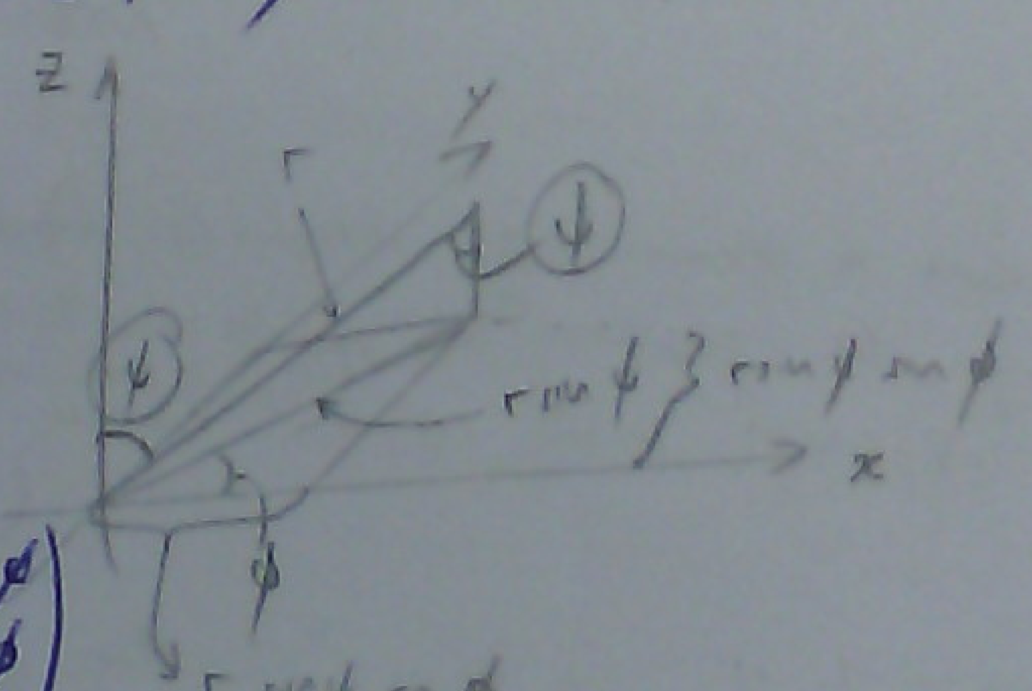
consider $D$ as in (*)

Then $S = [0,R] \times [0,2\pi)$ for bijection, as $0, 2\pi$ for sine/cos function maps to the same value.

(b) $u = r$

$v = \phi$

$w = \psi$



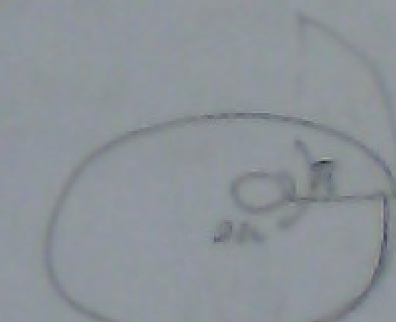

$x = r\sin\psi\cos\phi$

$y = r\sin\psi\sin\phi$

$z = r\cos\psi$

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = \Big[ \quad ? \quad \Big] \begin{bmatrix} dr \\ d\psi \\ d\phi \end{bmatrix}$$

$$\Phi(r,\phi,\psi) = \begin{pmatrix} r\sin\psi\cos\phi \\ r\sin\psi\sin\phi \\ r\cos\psi \end{pmatrix}$$




$\psi$ $\quad$ $\phi$

$D := \{(x,y,z) : x^2+y^2+z^2 \leq R^2\}$ $\quad S := [0,R] \times [0,\pi] \times [0,2\pi]$

$$\int_D dx\, dy\, dz = \int_S |\det \Phi'|\, dr\, d\phi\, d\psi$$

$u$

$x$

Example.

ⓐ $\Phi(r,\phi) = \begin{pmatrix} r\cos\phi \\ r\sin\phi \end{pmatrix}$

$\Phi'(r,\phi) = \begin{pmatrix} \cos\phi & -r\sin\phi \\ \sin\phi & r\cos\phi \end{pmatrix}$

$\det \Phi' = r(\cos^2\phi + \sin^2\phi)$

$= r$

$\Rightarrow \int_D dx\,dy = \int_0^{2\pi}\int_0^R r\,dr\,d\phi$

$= 2\pi \int_0^R r\,dr$

$= \pi\left[\frac{1}{2}r^2\right]_0^R$

$= \pi R^2$

ⓑ $\Phi(r,\psi,\phi) = \begin{pmatrix} r\sin\psi\cos\phi \\ r\sin\psi\sin\phi \\ r\cos\psi \end{pmatrix}$ $\quad \Phi'(r,\psi,\phi) = \begin{pmatrix} \sin\psi\cos\phi & r\cos\psi\cos\phi & -r\sin\psi\sin\phi \\ \sin\psi\sin\phi & r\cos\psi\sin\phi & r\sin\psi\cos\phi \\ \cancel{r}\cos\psi & -r\sin\psi & 0 \end{pmatrix}$

$\det \Phi'(r,\psi,\phi) = r^2\cos\psi(\cancel{r}\cos\psi\sin\psi\cos^2\phi + \sin\psi\cos\psi\sin^2\phi)$

$+ r^2\sin\psi(\sin^2\psi\cos^2\phi + \sin^2\psi\sin^2\phi)$

$= r^2(\cos^2\psi\sin\psi + \sin\psi\sin^2\psi)$

$= r^2\sin\psi$

$\rightarrow dx\,dy\,dz = \cancel{2\,dr}\, r^2\sin\psi\,dr\,d\psi\,d\phi$

## ② Recursion formulae

for : $\int_0^\infty x^n e^{-ax^2}dx =: I_n$

① $I_0 = \int_0^\infty e^{-ax^2}dx$

formally, to proceed, we need to determine if the integral is finite. in $e^{-x}$ form, at infinity, the polynomial $x^n$ will be cancelled entirely, at $x=0$, polynomial cancels out $e^{-x}$ function so it is finite!

$I_0^2 = \int_0^\infty e^{-ax^2}dx \int_0^\infty e^{-ay^2}dy$

$x = r\cos\phi$
$y = r\sin\phi$

$0 \to y \to \infty$
$0 \to x \to \infty$

$\cos\phi / \sin\phi \in [-1,1]$, but in our integration domain, $[0,\infty]$

$\cos\phi \to [0,1]$
$\Rightarrow \phi \to [0,\frac{\pi}{2}]$

$\Rightarrow = \int_0^\infty\int_0^\infty e^{-a(x^2+y^2)}dx\,dy$

$= \int_0^{\frac{\pi}{2}}\int_0^\infty e^{-ar^2}r\,dr\,d\phi$

$= \frac{\pi}{2}\int_0^\infty e^{-ar^2}r\,dr$ (**)

$z = ar^2 \quad dz = 2ar\,dr$

$= \frac{\pi}{2}\frac{1}{2a}\int_0^\infty e^{-z}dz = \frac{\pi}{4a}(-e^{-z})\Big|_0^\infty = \frac{\pi}{4a} \Rightarrow I_0 = \frac{1}{2}\sqrt{\frac{\pi}{a}}$

3

(ii) $I_1 = \int_0^\infty x e^{-ax^2}\,dx \overset{**}{=} \frac{1}{2a}$

$\int_0^\infty r^{?} e^{-ar^2}\,dr$ previously! $\Rightarrow \frac{1}{2a}$

(iii) Consider:

$$\frac{d}{da} I_n = \frac{d}{da}\int_0^\infty x^n e^{-ax^2}\,dx$$

$$= \int_0^\infty x^n \frac{d}{da} e^{-ax^2}\,dx$$

$$= -\int_0^\infty x^{n+2} e^{-ax^2}\,dx = -I_{n+2}$$

Index shift: recursion!

$$\boxed{I_n = \cancel{-\frac{d}{da}} - \frac{d}{da} I_{n-2} \qquad n = 2, 3, 4, \ldots}$$

Example:

$I_2 = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}$

$I_3 = \frac{1}{2a^2}$

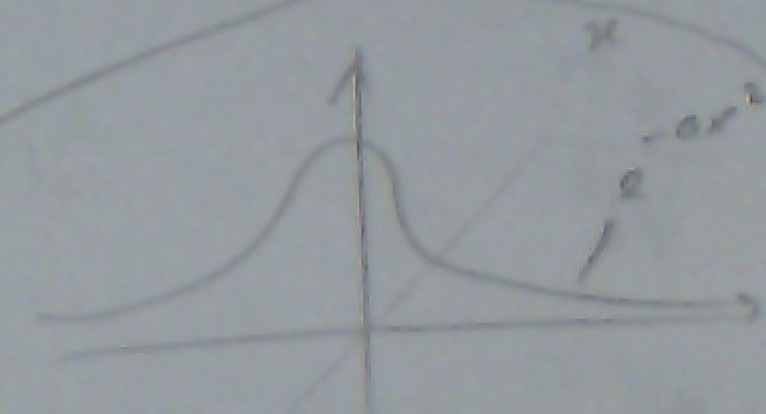
$I_4 = \frac{3}{8}\sqrt{\frac{\pi}{a^5}}$

Remark: $\tilde{I}_n = \int_{-\infty}^{\infty} x^n e^{-ax^2}\,dx$

$\tilde{I}_n = 0$ (n odd)

$\tilde{I}_n = 2 I_n$ (n even)

$x \cdot e^{-ax^2}$, the resulting product is an inverted left/right side. Integrating the whole domain cancels the left/right side exactly




(3) gaussian / maxwellian

Let $\hat{f}(c)$ be p.d.f.

normalise

$f(c) = n \hat{f}(c)$ — number density, $[n] = m^{-3}$

Note:

$n = \int_{\mathbb{R}^3} f(c)\,dc$ (velocity space) as $1 = \int_{\mathbb{R}^3} \hat{f}(c)\,dc$

We define:

expectation value of velocity gives a factor of $n$, so $\frac{1}{n}$ is there to normalize it!

$\underline{u}\cancel{x} \overset{A}{=} \frac{1}{n}\int_{\mathbb{R}^3} c\, f(c)\,dc$ "bulk velocity"

$$\frac{3}{2} k_B T = \frac{1}{n}\int_{\mathbb{R}^3} \frac{m}{2}\underbrace{|u-c|^2}_{\text{"thermal velocities"}} f(c)\,dc$$

Tomorrow: In equilibrium

$$f(c) = A e^{-\beta^2 |c - \alpha|^2}$$

Consider

$$n \doteq \int_{\mathbb{R}^3} f(\underline{c})\, d\underline{c} \qquad f(\underline{c}) = A\, e^{-\beta^2 |\underline{c} - \underline{\alpha}|^2}$$

$$\underline{\xi} = \underline{c} - \underline{\alpha} \qquad d\underline{\xi} = d\underline{c} \qquad d\underline{\xi} = [d\xi_1, d\xi_2, d\xi_3]$$

$$\Rightarrow n = \int_{\mathbb{R}^3} f(\underline{\xi})\, d\xi \qquad e^{-\beta^2\xi_1^2}\, e^{-\beta^2\xi_2^2}\, e^{-\beta^2\xi_3^2}$$

$$= A \int_{\mathbb{R}^3} e^{-\beta^2 \{\xi_1^2 + \xi_2^2 + \xi_3^2\}}\, d\xi_1\, d\xi_2\, d\xi_3$$

$$= A \underbrace{\left( \int_{\mathbb{R}} e^{-\beta^2 \xi^2} d\xi \right)^3}_{I_0 \;(a=\beta^2)}$$

$$\rightarrow \boxed{I_0 = \frac{\pi^{3/2}}{|\beta|^3}}$$

$$\Rightarrow n = A \cdot \frac{\pi^{3/2}}{|\beta|^3}$$

$$\Rightarrow A = \frac{n |\beta|^3}{\pi^{3/2}}$$

Ex: work out $\alpha = u$ using (4)

**Also:** $$\frac{3}{2} k_B T = \frac{m}{2} A \int_{\mathbb{R}^3} \xi^2 e^{-\beta^2 \xi^2}\, d\underline{\xi}$$

$$= \frac{m}{2} A \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \xi^4 e^{-\beta^2\xi^2} \sin\psi\, d\psi\, d\phi\, d\xi$$

$$\Rightarrow 3 k_B T = m A \cdot 2\pi \underbrace{\int_0^{\pi} \sin\psi\, d\psi}_{= -\cos\psi|_0^{\pi} = 2} \underbrace{\int_0^{\infty} \xi^4 e^{-\beta^2\xi^2} d\xi}_{= I_4 \;(a=\beta^2)}$$

$$I_4 = \frac{3}{8} \sqrt{\frac{\pi}{|\beta|^5}}$$

$$\beta^2 = \frac{m}{2 k_B T} \rightarrow, \quad A = \frac{n}{(2\pi R T)^{3/2}}$$

$$k_B = \frac{\hat{R}}{N_A} = \frac{RM}{N_A} = R \cdot m$$

Maxwell - Boltzmann

$$f(\underline{c}) = \frac{n}{(2\pi R T)^{3/2}}\, e^{\left(-\frac{|\underline{c} - \underline{u}|^2}{2RT}\right)}$$

Compare to standard gaussian:

$$N^3(\mu, \sigma) = \frac{1}{(2\pi)^{3/2} \sigma^3} \exp\left\{ \frac{-|\underline{x} - \underline{\mu}|^2}{2\sigma^2} \right\}$$

$\sigma^2 = RT$

$\mu_i = u_i, \; i = 1, 2, 3.$

LBM ~~4th Oct 2015~~ 4th Nov 2016



(4.2) Equilibrium velocity distribution

1. basic definitions

Postulate ~~$\hat{f}(c)$~~ $\hat{f}(\underline{c})$ (molecular velocities) such that

$$\int_{\mathbb{R}^3} \hat{f}(\underline{c}) \underbrace{dc_1\, dc_2\, dc_3}_{d\underline{c}} = 1$$

Hence $\hat{f}(\underline{c})\,d\underline{c}$ is probability that a molecule has velocity between $c_i$ and $c_i + dc_i$ $(i = 1, 2, 3)$

We use:

$$f(\underline{c}) = n \hat{f}(\underline{c}) \quad \rightarrow \rho = m \cdot n$$ (mass of molecule)

We define:

$$\underline{u} = \frac{1}{n}\int_{\mathbb{R}^3} \underline{c} f(\underline{c})\, d\underline{c} = 0$$ (under equilibrium assumption)

$$\frac{3}{2} k_B T = \int_{\mathbb{R}^3} \frac{m}{2} |u - c|^2 f(\underline{c})\, d\underline{c}$$

$$= \int_{\mathbb{R}^3} \frac{m}{2} \xi^2 f(\xi)\, d\xi \; ; \; \xi = \underline{c} - \underline{u} \; , \; \xi^2 = |\xi|^2$$

2. How to find $f$ ?

Equilibrium assumption : $\frac{\partial}{\partial t}\{f(\underline{c})\,d\underline{c}\} = 0$ ($f \neq f(x)$)

* only mechanism changing $f(\underline{c})$: collisions.
* $\underbrace{\text{"depleting" collisions}}_{\text{I}}$ and $\underbrace{\text{"replenishing" collisions}}_{\text{II}}$

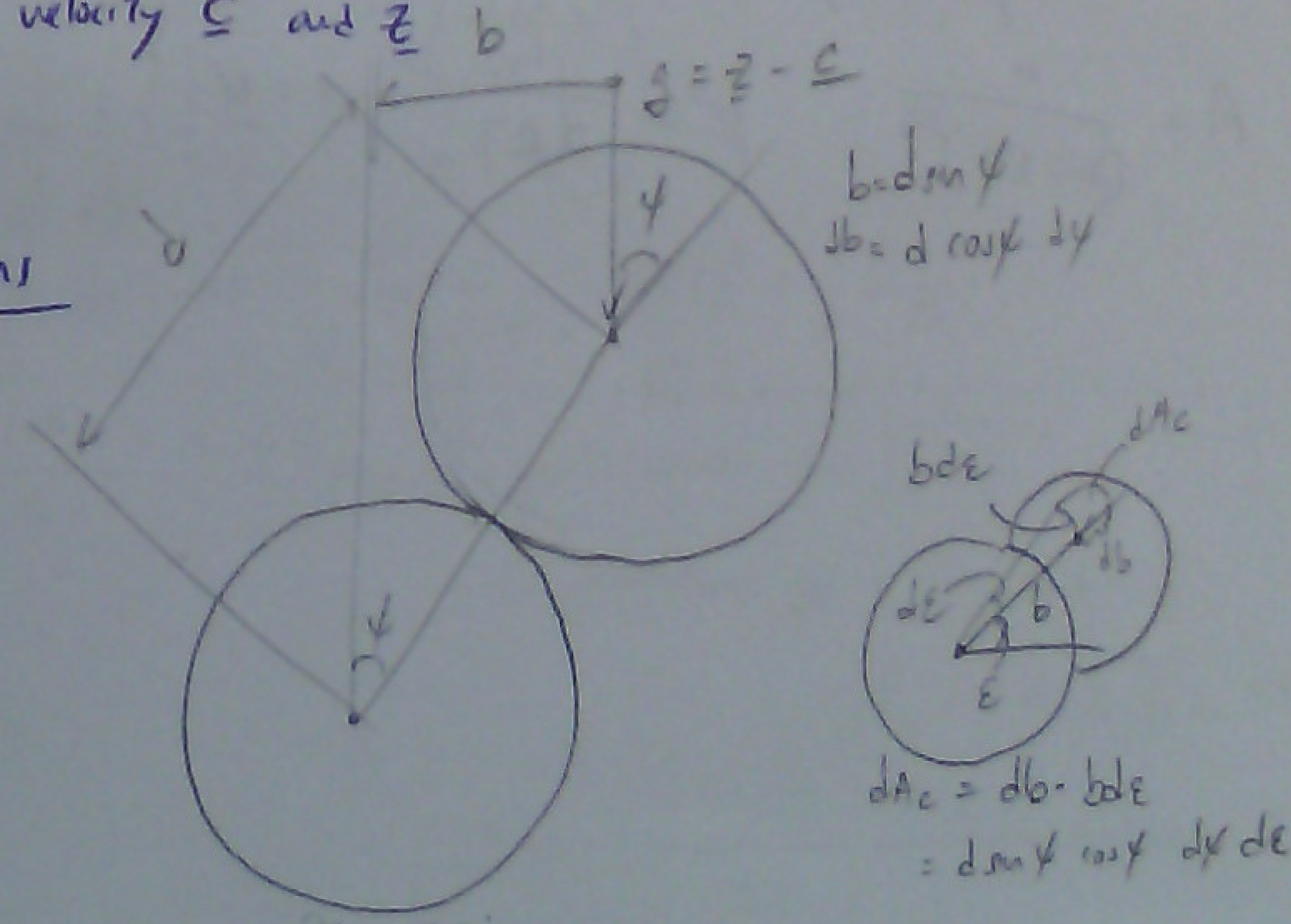
I. Consider collision between molecules having velocity $\underline{c}$ and $\underline{z}$ b

A priori assumption

$$\frac{\partial}{\partial t}\{f(\underline{c})\,d\underline{c}\} \propto f(\underline{c})\,d\underline{c} \times \frac{\#\text{ collisions}}{dt}$$

more molecule that travel in velocity $c$, more chance of collision with other velocity $z$, more rate of change

We reference frame with velocity $\underline{c}$:



$dV_c := \underbrace{g\,dt}_{\text{distance travelled}} \, dA_c$ } unit area = volume covered by particle moving in velocity $g = z - c$

All particle (with velocity $\underline{z}$) inside $dV_c$

i.e. $f(z)\,dz\,dV_c$

will hit our particle with velocity $\underline{c}$ during

$$\Rightarrow \frac{\partial f(c)\,dc}{\partial t} \; (2) = \int_{\mathbb{R}^3}\int_0^{\pi/2}\int_0^{2\pi} d^2\, \underbrace{g(c,\underline{z})}_{\text{norm}} f(\underline{c}) f(\underline{z}) \sin\psi \cos\psi \, d\psi\, d\varepsilon\, dc\, d\underline{z}$$

norm, hence $c/\underline{z} = -(c/\underline{z})$ doesn't matter the direction (+/-). symmetry, hence $\int_0^{\pi} \to \int_0^{\pi/2}$ for $d\psi$

$$\Rightarrow \frac{\partial\{f(c)\,dc\}}{\partial t} \; (1) = \int_{\mathbb{R}^3}\int_0^{\pi/2}\int_0^{2\pi} d^2\, g(c',z')\, f(\underset{\Downarrow}{c'}) f(z') \sin\psi\cos\psi\, d\psi\, d\varepsilon\, dz'\, dc'$$

$\underline{F}_1(c,\underline{z})$ — collision change of velocity function!

$$= \int_{\mathbb{R}^3}\int_0^{\pi/2}\int_0^{2\pi} d^2\, g(c,\underline{z})\, f(\underline{F}_1(\underline{c},\underline{z})) f(\underline{F}_2(c,\underline{z})) \sin\psi\cos\psi\, d\psi\, d\varepsilon\, d\underline{z}\, d\underline{c}\, \overbrace{|\det F'|}^{=1}$$

$$\to \frac{\partial f(c)}{\partial t} = \iiint g(c,\underline{z}) \Big( \underbrace{f(\overbrace{F_1(\underline{c},\underline{z})}^{c'}) f(\overbrace{F_2(\underline{c},\underline{z})}^{z'}) - f(c) f(\underline{z})}_{\substack{\text{desired balanced}\\ = 0}} \Big) \overbrace{dA_c}^{d^2\sin\psi\cos\psi\,d\psi\,d\varepsilon}\, d\underline{z}$$

note, we don't integrate over $dc$, because we only account for particles in $c$ velocity.

$$\to f(c') f(\underline{z}') = f(c) f(\underline{z})$$

$$\log f(c') + \underbrace{\log f(\underline{z}') = \log}_{\text{before \& after collisions, a quantity must be conserved}} f(c) + \log f(\underline{z})$$

So $\log f(c)$ must be of the form

that means $\log f(c)$ is a linear combination of conserved quantities, that is mass ($m$), momentum ($m\underline{v}$), energy ($\frac{m}{2}v^2$)

$$\log f(c) = a + b_1 c_1 + b_2 c_2 + b_3 c_3 + \frac{\tilde{a}}{2}|\underline{c}|^2$$

in other words, $\log f(c) = \operatorname{span}\{1, \underset{\text{velocity}}{\underline{v}}, \frac{|v|^2}{2}\}$

$$= -\beta^2\left((c_1-\alpha_1)^2 + (c_2-\alpha_2)^2 + (c_3-\alpha_3)^2\right) + \alpha_0$$

$$\Rightarrow f(c) = e^{-\beta^2|c-\underline{\alpha}|^2}\, e^{\alpha_0} = A$$

We showed yesterday:

$$A = \frac{n}{(2\pi RT)^{3/2}} \qquad \beta^2 = \frac{1}{2RT} \qquad \underline{\alpha} = \underline{u}$$

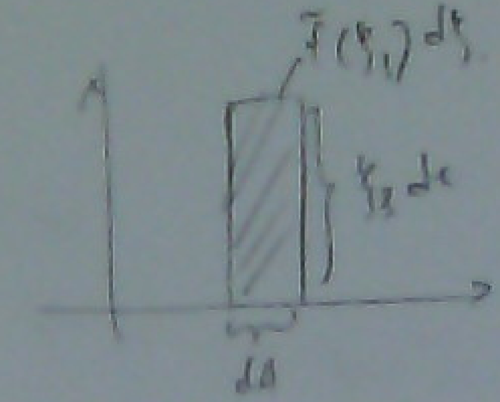
Note! The whole derivation of $f(c)$ in this lecture is dependent on the assumption that the gas is in equilibrium! If the assumption doesn't hold, then $f(c)$ is unknown!

define pressure as mean momentum flux of "thermal" momentum.

$m\xi = m(\xi_1, \xi_2, \xi_3)^T$

$f(c) = A_e^{-\beta^2 |c-u|^2}$

$\tilde{f}(\xi) = A_e^{-\beta^2 |\xi|^2}$




Assume: Equilibrium $f$ is Maxwellian

Winter Semester 2016/17

# Lattice-Boltzmann Methods

Prof. Georg May

Tutorial 3

$dM = m\xi_3 \tilde{f}(\xi_1)\xi_1 dt\, dA\, d\xi_1\, d\xi_2\, d\xi_3$ "momentum"

$P_1 := \int m\xi_1^2 \tilde{f}(\xi_1) d\xi_3\, d\xi_2\, d\xi_1$ $\quad \frac{3}{2} n k_B T$

$P := \frac{1}{3}(P_1 + P_2 + P_3) = \frac{2}{3}\int \frac{m}{2}|\xi|^2 \tilde{f}(\xi_1)\, d\xi$

## Problem 1

Derive an expression for the thermodynamic pressure as the mean flux of the molecular "thermal" momentum $m\boldsymbol{\xi}$. (Here $\boldsymbol{\xi} = \mathbf{c} - \mathbf{u}$ is the thermal vecocity, given by the difference between the molecular velocity $\mathbf{c}$ and the bulk fluid velocity $\mathbf{u}$.)

## Problem 2

Compute the mean velocity *magnitude* for a gas in thermodynamic equilibrium from the Maxwell-Boltzmann distribution.

## Problem 3

Compute the mean free path of a molecule of a gas in thermodynamic equilibrium, using the Maxwell-Boltzmann distribution.

Problem 2:

we use $\hat{f} = \frac{1}{n} f$

$\hat{f}(c) = \frac{1}{(2\pi RT)^{3/2}} \int_{\mathbb{R}^3} e^{-\frac{|c|^2}{2RT}} dc$

$\bar{c} = \langle |c| \hat{f}(c) \rangle$

$= \frac{1}{(2\pi RT)^{3/2}} \int_{\mathbb{R}^3} |c|\, e^{-\frac{|c|^2}{2RT}} dc$, convert to spherical coord.

$|c|^2$ can be thought as the product of vector $c = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ or $\begin{bmatrix} c\sin\psi\cos\phi \\ c\sin\psi\sin\phi \\ c\cos\psi \end{bmatrix}$

spherical coordinates:

$dc_1\, dc_2\, dc_3 = dc = c^2 \sin\psi\, d\phi\, d\psi\, dc$

$\Rightarrow \bar{c} = \frac{1}{(2\pi RT)^{3/2}} \underbrace{\int_0^\infty c^3 e^{-\frac{c^2}{2RT}} dc}_{I_3\left(\frac{1}{2RT}\right)} \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \underbrace{\int_0^\pi \sin\psi\, d\psi}_{2} \Rightarrow \frac{4\pi}{(2\pi RT)^{3/2}} 2(RT)^2 = \sqrt{\frac{8RT}{\pi}}$

Compare: speed of sound: $c = \sqrt{\gamma RT}$

For monoatomic gas: $\gamma = 1.666 = \frac{5}{3}$

$\sqrt{\frac{8}{\pi}} = 1.6 \;\&\; \sqrt{\frac{5}{3}} = 1.3$

$I_n(a) = \int_0^\infty x^n e^{-ax^2} dx \quad (a > 0)$

$I_3(a) = -\frac{d}{da} I_1(a) = -\frac{d}{da}\left(\frac{1}{2a}\right) = \frac{1}{2a^2} = 2(RT)^2$

Problem 3

$$\frac{1}{n}\int_{\mathbb{R}^3} \frac{\partial f(\xi)\, d\xi}{\partial t}\Bigg|_I =: \upsilon \text{, no. of collisions per unit time}$$

collision tube: $d^2 \sin\psi\cos\psi\; d\epsilon\, d\psi$

$$\upsilon = \frac{1}{n}\int_{A_c}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g(\xi,z)\, f(\xi)\, f(z)\, \overbrace{dA_c}\, dz\, d\xi$$

Since $f$ is Maxwellian:

$$= \frac{1}{n}\frac{n^2 d^2}{(2\pi RT)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_0^{2\pi}\int_0^{\pi/2} g(\xi,z)\, e^{-\frac{|\xi|^2+|z|^2}{2RT}} \sin\psi\cos\psi\; d\psi\, d\epsilon\, d\xi\, dz$$

$$\int_0^{\pi/2}\sin\psi\cos\psi\, d\psi = \sin^2\psi\Big|_0^{\pi/2} \overbrace{- \int_0^{\pi/2}\sin\psi\cos\psi\, d\psi}^{\text{move to LHS}}$$

$$= \frac{1}{2}\sin^2\psi\Big|_0^{\pi/2} = \frac{1}{2}$$

$$\int_0^{2\pi} d\epsilon = 2\pi$$

$$\Rightarrow \upsilon = \frac{n d^2}{(2\pi RT)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g(\xi,z)\, e^{-\frac{|\xi|^2+|z|^2}{2RT}}\, d\xi\, dz \quad ; \; g = |\mathbf{g}| \text{, magnitude of } z-\xi = \mathbf{g}$$

Consider:

$g = z - \xi \Rightarrow z = g + \xi$ (a)

$\boxed{w = \frac{1}{2}(z+\xi)} = \frac{1}{2}(g+2\xi)$

$\Rightarrow \xi = w - \frac{1}{2}g$ (b)

substitute (b) into (a)

$\Rightarrow z = w + \frac{1}{2}g$ (c)

$F: \mathbb{R}^6 \to \mathbb{R}^6$

$$F(w,g) = \begin{pmatrix} F_1(w,g) \\ F_2(w,g) \end{pmatrix} \begin{matrix}(b)\\(c)\end{matrix} \qquad \begin{matrix}\xi = F_1(w,g) \\ z = F_2(w,g)\end{matrix}$$

3x3 Mat.

$$F' = \begin{pmatrix} \frac{\partial \xi}{\partial w} & \frac{\partial \xi}{\partial g} \\ \frac{\partial z}{\partial w} & \frac{\partial z}{\partial g} \end{pmatrix} = \begin{pmatrix} I & -\frac{1}{2}I \\ I & \frac{1}{2}I \end{pmatrix}$$

$$|\det F'| = \left|\det\left(\tfrac{1}{2}I + \tfrac{1}{2}I\right)\right| = 1$$

Now: $|\xi|^2 + |z|^2 = (w - \frac{1}{2}g,\, w-\frac{1}{2}g) + (w+\frac{1}{2}g,\, w+\frac{1}{2}g)$

$= 2|w|^2 + \frac{1}{2}|g|^2$

$$\upsilon = \frac{nd^2}{(2\pi RT)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} g\, e^{-\frac{(2|w|^2+\frac{1}{2}|g|^2)}{2RT}}\, dg\, dw \Rightarrow \underset{(d)}{\int_{\mathbb{R}^3} g\, e^{-\frac{|g|^2}{4RT}}\, dg} \; \underset{(e)}{\int_{\mathbb{R}^3} e^{-\frac{|w|^2}{RT}}\, dw}$$

$$(d) = 4\pi\underbrace{\int_0^\infty g^3 e^{-\frac{g^2}{4RT}}\, dg}_{I_3\left(\frac{1}{4RT}\right)} = 8(RT)^2 \qquad (e) = 4\pi\underbrace{\int_0^\infty w^2 e^{-\frac{w^2}{RT}}\, dw}_{I_2\left(\frac{1}{RT}\right)} = (\pi RT)^{3/2}$$

$\Rightarrow \upsilon = 4nd^2\sqrt{\pi RT}$ ; time between collisions, $\tau = \frac{1}{\upsilon}$ | $\lambda = \bar{c}\tau = \bar{c}/\upsilon = \sqrt{\frac{8RT}{\pi}}\cdot\frac{1}{\upsilon} = \frac{1}{\sqrt{2}\,\pi n d^2}$

## Chapter 5: The Boltzmann Equation.

In the non-equilibrium case.

$$f = f(\underline{c}, \underline{x}, t)$$

$$n(x,t) = \int_{\mathbb{R}^3} f(\underline{c}, \underline{x}, t)\, d\underline{c}$$

normalisation coefficient

$$u(x,t) = \frac{1}{n(x,t)} \int_{\mathbb{R}^3} \underline{c}\, f(\underline{c}, \underline{x}, t)\, d\underline{c}$$

Boltzmann Equation

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = J(f,f)$$

$$J(f,f) = \int_{A_c} \int_{\mathbb{R}^3} g(\underline{c}, \underline{z}) \left( f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z}) \right) dA_c\, d\underline{z}$$

<u>Can show:</u>

$$\int_{\mathbb{R}^3} \phi(\underline{c})\, J(f,f)\, d\underline{c} = 0 \quad ; \left( J(f,f) \sim \left.\frac{\partial f}{\partial t}\right|_{coll.} \right)$$

$$\text{for } \phi(\underline{c}) = \begin{cases} m \\ m\underline{c} \\ \frac{1}{2} m |\underline{c}|^2 \end{cases}$$

collisional invariants.

literally, there is not net change in the conserved quantities due to <u>collision</u>

Take moments of Boltzmann Equations:

$$\int_{\mathbb{R}^3} \phi(\underline{c}) \left\{ \frac{\partial f}{\partial t} + \underbrace{c_\alpha \frac{\partial f}{\partial x_\alpha}}_{\text{einstein notation}} - J(f,f) \right\} d\underline{c} = 0$$

① $\phi(\underline{c}) = m$

$$\Rightarrow \int_{\mathbb{R}^3} \phi(\underline{c}) \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} d\underline{c} = 0$$

$$\Rightarrow \int_{\mathbb{R}^3} m \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} d\underline{c} = 0$$

$$\Rightarrow \frac{\partial}{\partial t} m \underbrace{\int_{\mathbb{R}^3} f(\underline{c})\, d\underline{c}}_{n} + \frac{\partial}{\partial x_\alpha} m \underbrace{\int_{\mathbb{R}^3} c_\alpha f(\underline{c})\, d\underline{c}}_{n u_\alpha} = 0$$

$\rho = m \cdot n$ look above!

$$\rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\alpha} (\rho u_\alpha) = 0$$

(ii) $\phi(\underline{c}) = m c_\alpha$

$$\Rightarrow \int_{\mathbb{R}^3} m c_\alpha \left( \frac{\partial f}{\partial t} + c_\beta \frac{\partial f}{\partial x_\beta} \right) d\underline{c} = 0$$

indices, as it indicates a tensor.

$$\Rightarrow \frac{\partial}{\partial t} m \underbrace{\int_{\mathbb{R}^3} c_\alpha f(c)\, d\underline{c}}_{n u_\alpha} + \frac{\partial}{\partial x_\beta} m \int_{\mathbb{R}^3} c_\alpha c_\beta f(c)\, d\underline{c} = 0$$

Recall: $\underline{c} = \underline{u} + \underline{\xi}$

$$\Rightarrow \frac{\partial}{\partial t}(\rho u_\alpha) + \frac{\partial}{\partial x_\alpha} m \int_{\mathbb{R}^3} (u_\alpha + \xi_\alpha)(u_\beta + \xi_\beta) \tilde{f}(\xi)\, d\xi = 0$$

(deviation) 0, average of deviation de velocity $\Rightarrow 0$ (Check!)

$$\Rightarrow \frac{\partial}{\partial t}(\rho u_\alpha) + \frac{\partial}{\partial x_\alpha} m \Big\{ \underbrace{\int_{\mathbb{R}^3} u_\alpha u_\beta \tilde{f}(\xi)\, d\xi}_{n} + \int_{\mathbb{R}^3} \xi_\alpha u_\beta \tilde{f}(\xi)\, d\xi + \int_{\mathbb{R}^3} u_\alpha \xi_\beta \tilde{f}(\xi)\, d\xi + \underbrace{\int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \tilde{f}(\xi)\, d\xi}_{P_{\alpha\beta} = m \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \tilde{f}(\xi)\, d\xi} \Big\} = 0$$

$\int_{\mathbb{R}^3} \xi_\alpha \tilde{f}(\xi)\, d\xi = 0$

expectation value of velocity fluctuations

(iii) $\phi(\underline{c}) = \frac{1}{2} m c^2$

$$\int_{\mathbb{R}^3} \frac{1}{2} m c^2 \left\{ \frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} \right\} d\underline{c} = 0$$

$$\underbrace{\frac{\partial}{\partial t} \frac{1}{2} m \int_{\mathbb{R}^3} c^2 f(c)\, d\underline{c}}_{(a)} + \underbrace{\frac{\partial}{\partial x_\alpha} \frac{1}{2} m \int_{\mathbb{R}^3} c^2 c_\alpha f(c)\, d\underline{c}}_{(b)} = 0$$

Note: $c^2 = (\underline{u} + \underline{\xi}, \underline{u} + \underline{\xi})$

$= \underline{u}^2 + 2(\underline{\xi}, \underline{u}) + \xi^2$

$$(a) = \frac{\partial}{\partial t} \frac{m}{2} \int_{\mathbb{R}^3} (u^2 + \xi^2) f(\xi)\, d\xi$$

$$= \frac{\partial}{\partial t} \underbrace{\left( \frac{m}{2} n u^2 + \overbrace{\int \frac{m}{2} \xi^2 f(\xi)\, d\xi}^{= \frac{3}{2} n k_B T} \right)}_{E}$$

$$(b)\ \frac{\partial}{\partial x_\beta} \left\{ \frac{m}{2} \int_{\mathbb{R}^3} (\xi_\beta + u_\beta)(u^2 + 2\xi_\alpha u_\alpha + \xi^2) f(\xi)\, d\xi \right\}$$

$P_{\alpha\beta} u_\alpha$, $q_\beta$

$$= \frac{\partial}{\partial x_\beta} \Big\{ \frac{m}{2} \int_{\mathbb{R}^3} 2 \xi_\alpha \xi_\beta u_\alpha f(\xi)\, d\xi + \frac{m}{2} \int_{\mathbb{R}^3} \xi_\beta \xi^2 f(\xi)\, d\xi + \underbrace{\frac{m}{2} u^2 u_\beta \underbrace{\int_{\mathbb{R}^3} f(\xi)\, d\xi}_{n} + \underbrace{\frac{m}{2} \int_{\mathbb{R}^3} u_\beta \xi^2 f(\xi)\, d\xi}_{u_\beta \cdot \frac{3}{2} n k_B T}}_{E u_\beta} \Big\}$$

$$(a) + (b) \Rightarrow \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_\beta}(E u_\beta) + \frac{\partial}{\partial x_\beta}(P_{\alpha\beta} u_\alpha) + \frac{\partial q_\beta}{\partial x_\beta} = 0$$

Assume: Local thermodynamic equilibrium

$$f(\underline{c}, \underline{x}, t) = \frac{n(x,t)}{(2\pi R T(x,t))^{3/2}} e^{\frac{-|c - u(x,t)|^2}{2RT(x,t)}}$$

Consider:

$$P_{\alpha\beta} = \int_{\mathbb{R}^3} m \xi_\alpha \xi_\beta f(\xi)\, d\xi = \overbrace{\frac{nm}{(2\pi RT)^{3/2}}}^{A} \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta e^{\frac{-|\xi|^2}{2RT}}\, d\xi$$

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(i) $\alpha \neq \beta$

$$P_{\alpha\beta} = A \int_{\mathbb{R}^3} \xi_\alpha e^{-\frac{\xi_\alpha^2}{2RT}} d\xi \int_{\mathbb{R}^3} \xi_\beta e^{-\frac{\xi_\beta^2}{2RT}} d\xi \int_{\mathbb{R}^3} e^{-\frac{\xi_\gamma^2}{2RT}} d\xi$$

$\rightarrow 0$, mean zero!

$$(\alpha, \beta, \gamma) = \sigma(1, 2, 3)$$ permutation

$$P_{\alpha\beta} = 0 \quad (\alpha \neq \beta)$$

(ii) $\alpha = \beta$

$$P_{\alpha\alpha} = A \int_{\mathbb{R}^3} m \xi_\alpha^2 e^{-\frac{\xi_1^2+\xi_2^2+\xi_3^2}{2RT}} d\xi$$

$$= \underbrace{\frac{A}{3} \int_{\mathbb{R}^3} m \underbrace{(\xi_1^2 + \xi_2^2 + \xi_3^2)}_{\xi^2} e^{-\frac{\xi^2}{2RT}} d\xi}_{P}$$

$$\Rightarrow q_\beta = \int \frac{m}{2} \xi^2 \xi_\beta f(\xi) d\xi$$

$$= \frac{\rho}{(2\pi RT)^{3/2}} \int_{\mathbb{R}^3} \xi^2 \xi_\beta e^{-\frac{\xi^2}{2RT}} d\xi$$

$h(\psi, \phi)$

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix} = \begin{pmatrix} \xi \sin\psi \cos\phi \\ \xi \sin\psi \sin\phi \\ \xi \cos\psi \end{pmatrix}$$

spherical coordinates:

$$q_\beta = A \iiint_{\rho\psi\phi} \xi^2 \underbrace{\xi \cdot h(\psi, \phi)}_{\xi_\beta} e^{-\frac{\xi^2}{2RT}} \xi^2 \sin\psi \, d\psi \, d\phi \, d\xi$$

$$\Rightarrow q_\beta = A \int_0^\infty \xi^5 e^{-\frac{\xi^2}{2RT}} \underbrace{\int_0^\pi \int_0^{2\pi} h(\psi, \phi) \sin\psi \, d\psi \, d\phi}_{(*)}$$

eg. $\beta = 2$, $h(\psi, \phi)_2 = \sin\psi \sin\phi$

$$\Rightarrow (*) = \int_0^\pi \sin^2\psi \, d\psi \underbrace{\int_0^{2\pi} \sin\phi \, d\phi}_{0}$$

$\beta = 3$

$$\Rightarrow (*) = \int_0^\pi \sin\psi \cos\psi \, d\psi = \frac{1}{2} \sin^2\psi \Big|_0^\pi = 0$$

hence $q = 0$, if $f$ is maxwellian.

$$\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_\alpha)}{\partial x_\alpha} = 0$$

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta} + \frac{\partial P}{\partial x_\alpha} = 0$$

$$\frac{\partial E}{\partial t} + \frac{\partial (E u_\beta)}{\partial x_\beta} + \frac{\partial p u_\beta}{\partial x_\beta} = 0$$

f is locally Maxwellian.

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Today:

1. Collisional invariants
2. Boltzmann H-theorem

1. Recall: Collision integral:

collision angle

$$J(f,f) = \int_{\mathbb{R}^3} \int_{A_c} g(\underline{c},\underline{z}) \left( f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z}) \right) d\underline{z}\, dA_c \quad ; \quad \underline{c}'(\underline{c},\underline{z};\psi,\varepsilon)$$

$$\underline{z}'(\underline{c},\underline{z};\psi,\varepsilon)$$

$$\underline{F} = \begin{pmatrix} \underline{F}_1(\underline{c},\underline{z};\psi,\varepsilon) \\ \underline{F}_2(\underline{c},\underline{z};\psi,\varepsilon) \end{pmatrix} \qquad \underline{F}_1' = \underline{c}' \qquad \underline{F}_2' = \underline{z}'$$

$$\underline{F}_1 = \underline{c} + 2\mu_B(\underline{g}, \underline{k}(\psi,\varepsilon))\, \underline{k}(\psi,\varepsilon)$$

$$\underline{F}_2 = \underline{z} - 2\mu_A(\underline{g}, \underline{k}(\psi,\varepsilon))\, \underline{k}(\psi,\varepsilon)$$

$$\mu_i = \frac{m_i}{m_A + m_B} \qquad i = A, B$$

$$m_A + m_B = \mu_i = \frac{1}{2}$$

Boltzmann Eqn:

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = J(f,f)$$

Consider moments:

$$I_\phi := \int_{\mathbb{R}^3} J(f,f)\phi(\underline{c})\, d\underline{c}$$

$$\rightarrow I_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(\underline{c},\underline{z})\left(f(\underline{c}')f(\underline{z}') - f(\underline{c})f(\underline{z})\right)\phi(\underline{c})\, d\underline{c}\, d\underline{z}\, dA_c \qquad (1)$$

Now, trivially exchange variable names $\underline{c} \leftrightarrow \underline{z}$

$$\rightarrow I_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(\underline{z},\underline{c})\left(f(\underline{c}'(\cdot))\, f(\underline{z}'(\cdot)) - f(\underline{z})f(\underline{c})\right)\phi(\underline{z})\, d\underline{c}\, d\underline{z}\, dA_c$$

$$\underline{c}' = \underline{c}'(\underline{z},\underline{c},\psi,\varepsilon)$$

$$\underline{z}' = \underline{z}'(\underline{z},\underline{c},\psi,\varepsilon)$$

Now consider physical symmetries

$$\underline{g}(\underline{c},\underline{z}) = -\underline{g}(\underline{z},\underline{c}) \qquad \text{also:} \quad \underline{c}'(\underline{c},\underline{z}) = \underline{z}'(\underline{z},\underline{c})$$

$$\Rightarrow g(\underline{c},\underline{z}) = g(\underline{z},\underline{c}) \qquad \underline{z}'(\underline{c},\underline{z}) = \underline{c}'(\underline{z},\underline{c})$$

$|\underline{g}|$

from *

(2)

$$\Rightarrow I_\phi = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} g(c,z)\left(f(c'(c,z))f(z'(c,z)) - f(c)f(z)\right)\phi(z)\,\cancel{\phi(c)}\,dc\,dz\,dA_c$$

We can now write:

$$I_\phi = \frac{1}{2}\left((1) + (2)\right)$$

Similarly can rewrite twice more

$$\Rightarrow I_\phi = \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{A_c} \cancel{g(c)}\, g(c,z)\left(f(c')f(z') - f(c)f(z)\right)\left(\phi(c) + \phi(z) - \phi(c') - \phi(z')\right) dc\,dz\,dA_c$$

see notes for derivation

$I_\phi = 0$ for $\phi(c)$ s.th $\phi(c) + \phi(z) = \phi(c') + \phi(z')$

true for: $\phi(c) = \begin{cases} m \\ m c \\ \frac{m}{2} c^2 \end{cases}$

## ② H - Theorem:

$$H = -\int_{\mathbb{R}^3} f \ln f \, dc \qquad \text{Assume } f = f(c,t)$$

We show

(i) $\frac{dH}{dt} \geq 0$ and $\frac{dH}{dt} = 0$ iff $f$ is Maxwellian.

(ii) $H$ is entropy.

---

(ii) Consider Entropy of closed system.

$T\,dS = dE + p\,dV$ (energy, pressure)

ideal gas != $p = n k_B T$

$= \frac{N}{V} k_B T$

$e = \frac{3}{2} n k_B T \Rightarrow E = eV$

$= \frac{3}{2} N k_B T$

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(2)

$$dS = \frac{3}{2} N k_B \frac{dT}{T} + N k_B \frac{dV}{V}$$ $\leftarrow$ $PV = nRT$, $P = \frac{N}{V} k_B T$

$$= N k_B \left( \frac{3}{2} \frac{dT}{T} + \frac{dV}{V} \right)$$

$$S - S_0 = N k_B \left( \frac{3}{2} \ln\left(\frac{T}{T_0}\right) + \ln\left(\frac{V}{V_0}\right) \right) \quad ; \; n = N/V, \; \frac{n}{n_0} = \frac{V_0}{V}$$

$$= N k_B \left( \frac{3}{2} \ln\left(\frac{T}{T_0}\right) - \ln\left(\frac{n}{n_0}\right) \right)$$

$$\Rightarrow S = N k_B \left( \frac{3}{2} \ln(T) - \ln(n) + C_0(N) \right)$$

## H-Function

$$f = \frac{n}{(2\pi k_B T)^{3/2}} e^{-\frac{c^2}{2RT}}$$

Maxwellian

$$H = -\int_{\mathbb{R}^3} f \ln f$$

$$= -\int_{\mathbb{R}^3} f \left( \ln(n) - \frac{3}{2} \ln(2\pi k_B T) - \underbrace{\frac{c^2}{2RT}}_{\frac{mc^2}{2k_B T}} \right) d\underline{c} \quad ; \; R = \frac{k_B}{m}$$

$$\Rightarrow \int \frac{m}{2} c^2 f \, d\underline{c} = \frac{3}{2} n k_B T$$

$$\frac{1}{n} \int_{\mathbb{R}^3} f \, d\underline{c} = 1$$

normalisation of f

$$\Rightarrow H = -n \ln(n) + \frac{3}{2} n \ln(T) + \frac{3}{2} \frac{k_B T}{k_B T} + C_1$$

$$= -n \left( \ln(n) - \frac{3}{2} \ln(T) \right) + \tilde{C}_1$$ note similarity with S above?

(.) Recall: $f \equiv f(\underline{c}, t)$

$$\Rightarrow \frac{\partial f}{\partial t} = J(f, f) \quad \text{(Boltzmann eqn.)}$$

$$\rightarrow \frac{\partial H}{\partial t} = -\frac{\partial}{\partial t} \int_{\mathbb{R}^3} f \ln f \, d\underline{c}$$

$$= -\int_{\mathbb{R}^3} \left( \frac{\partial f}{\partial t} \ln f + f \frac{1}{f} \frac{\partial f}{\partial t} \right) d\underline{c}$$

$$= -\int_{\mathbb{R}^3} \frac{\partial f}{\partial t} (1 + \ln f) \, d\underline{c}$$

$$= -\int_{\mathbb{R}^3} J(f, f) \ln f \, d\underline{c} - \underbrace{\int_{\mathbb{R}^3} J(f, f) \, d\underline{c}}_{0 \text{ (collisional invariants)}} = -I_\phi \quad ; \; \phi = \ln f(\underline{c})$$

$$\Rightarrow \frac{\partial H}{\partial t} = -\int_{\mathbb{R}^3} \partial(f,f)\big(\ln(f(c)) + \ln(f(z)) - \ln(f(c')) - \ln(f(z'))\big) J(f,f)\, dc$$

$$= -\int_{\mathbb{R}^3} g(c,z)\underbrace{\big(f(c')f(z') - f(c)f(z)\big)}_{\circledast} \underbrace{\ln\left(\frac{f(c)f(z)}{f(c')f(z')}\right)}_{\star} dc\, dz\, dA_c$$

if $\circledast > 0$, $\star < 0$, hence $\frac{\partial H}{\partial t} > 0$

if $\circledast < 0$, $\star > 0$, hence $\frac{\partial H}{\partial t} > 0$

$\Big\}$ always larger than 0, $= 0$ iff $\circledast = 0$.

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$$\frac{dy}{dt} = \frac{\bar{y} - y}{\tau} \quad (\tau > 0)$$

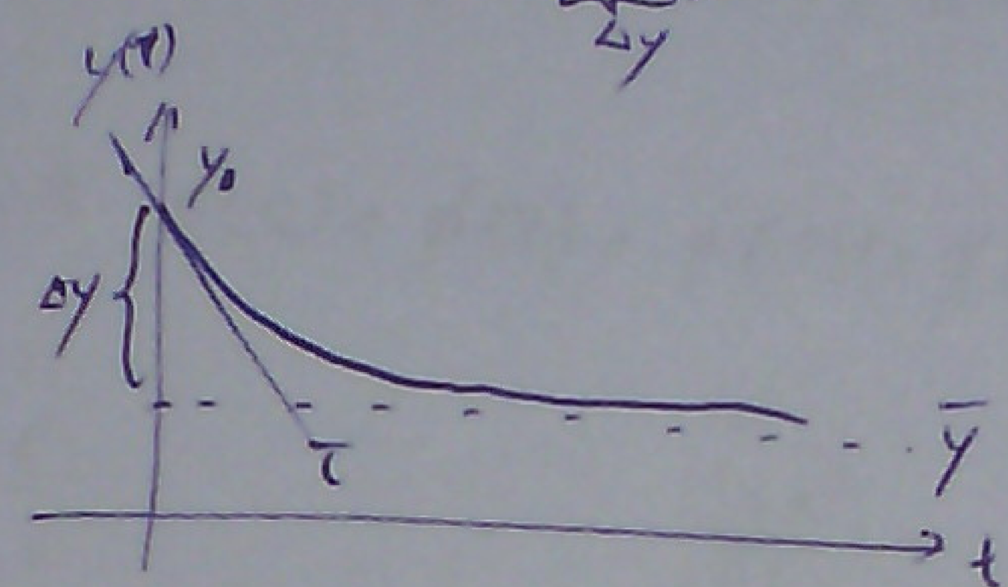
$$\int_{y_0}^{y} \frac{d\tilde{y}}{\bar{y} - \tilde{y}} = \int_0^t \frac{1}{\tau} d\tilde{t}$$

$$\rightarrow -\ln(\bar{y} - \tilde{y})\Big|_{y_0}^{y} = \frac{t}{\tau}$$

$$\rightarrow \ln \frac{\bar{y} - y}{\bar{y} - y_0} = \frac{-t}{\tau}$$

$$\Rightarrow \bar{y} - y = (\bar{y} - y_0)\, e^{-t/\tau}$$

$$y(t) := \bar{y} - \underbrace{(\bar{y} - y_0)}_{\Delta y} e^{-t/\tau}$$




The BGK Eqn:

Recall: $\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = J(f,f)$

BGK:

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{f^{(eq)} - f}{\tau}$$

Maxwellian

Dimensional analysis:

Example: Compressible (steady) N-S eqn.

$$\frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta}\Big\{\underbrace{\mu\Big(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial u_\beta}{\partial x_\beta}\Big)}_{\tau_{\alpha\beta}}\Big\}$$

dyn pressure $p + \frac{1}{2}\rho u^2 =$ const.

$$\tilde{\rho} = \frac{\rho}{\rho_\infty} \qquad \tilde{p} = \frac{p}{\rho_\infty u_\infty^2}$$

$$\tilde{u}_\alpha = \frac{u}{U_\infty} \qquad \tilde{x}_\alpha = \frac{x_\alpha}{L}$$

dimensionless

$$\frac{\rho_\infty u_\infty^2}{L}\frac{\partial(\tilde{\rho}\tilde{u}_\alpha\tilde{u}_\beta)}{\partial\tilde{x}_\beta} + \frac{\rho_\infty u_\infty^2}{L}\frac{\partial\tilde{p}}{\partial\tilde{x}_\alpha} = \frac{\mu u_\infty}{L^2}\frac{\partial}{\partial\tilde{x}_\beta}\Big(\frac{\partial\tilde{u}_\alpha}{\partial\tilde{x}_\beta} + \frac{\partial\tilde{u}_\beta}{\partial\tilde{x}_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial\tilde{u}_\beta}{\partial\tilde{x}_\beta}\Big)$$

$$\Rightarrow \frac{\partial(\tilde{\rho}\tilde{u}_\alpha\tilde{u}_\beta)}{\partial\tilde{x}_\beta} + \frac{\partial\tilde{p}}{\partial\tilde{x}_\alpha} = \underbrace{\frac{\mu}{\rho_\infty u_\infty L}}_{\frac{1}{Re}}(\dots)$$

Chapman - Enskog expansion

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Recall: BGK Equation → Non-Dimensionalize

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \frac{f^{(eq)} - f}{\tau} = (f^{(eq)} - f)\,\nu \quad ; \nu = \frac{1}{\tau}$$

$$\tilde{x}_\alpha = \frac{x_\alpha}{L} \qquad \tilde{t} = \frac{t}{L/\bar{c}} \qquad \bar{c} = \frac{1}{n}\int f(c)\,dc \;;\; c = \{c_1, c_2, c_3\}$$

$$\tilde{c}_\alpha = \frac{c_\alpha}{\bar{c}} \quad \text{average velocity} \qquad \tilde{f} = \frac{f\,\bar{c}^3}{n_0} \qquad f = \frac{n}{\bar{c}^3} \qquad \tilde{\nu} = \frac{\nu}{\nu_0} = \frac{\nu}{\bar{c}}\lambda$$

$$\Rightarrow \frac{n_0 \bar{c}}{\bar{c}^3 L}\frac{\partial \tilde{f}}{\partial \tilde{t}} + \bar{c}\frac{n_0}{\bar{c}^3}\tilde{c}_\alpha \frac{1}{L}\frac{\partial \tilde{f}}{\partial \tilde{x}_\alpha} = \frac{\bar{c}}{\lambda}\frac{n_0}{\bar{c}^3}\tilde{\nu}\,(\tilde{f}^{(eq)} - f)$$

$$\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}}{\partial \tilde{x}_\alpha} = \underbrace{\frac{L}{\lambda}}_{\text{mfp}}^{Kn}\,\tilde{\nu}\,(\tilde{f}^{(eq)} - \tilde{f})$$

set $Kn \equiv \varepsilon$

As $\varepsilon \to 0$ $f \approx f^{(eq)}$

Assume $\varepsilon \ll 1$

$$f = \underset{f^{(eq)}}{f_0} + \varepsilon f_1 + \varepsilon^2 f_2 + \varepsilon^3 f_3 + \dots$$
$$= \sum_{k=0}^{\infty} \varepsilon^k f_k$$

Substitute in BGK

$$\varepsilon\frac{\partial(\tilde{f}_0 + \varepsilon\tilde{f}_1 + \varepsilon^2\tilde{f}_2 + \dots)}{\partial t} + \varepsilon\tilde{c}_\alpha \frac{\partial(\tilde{f}_0 + \varepsilon\tilde{f}_1 + \varepsilon^2\tilde{f}_2 + \dots)}{\partial \tilde{x}_\alpha} = \tilde{\nu}\,(\tilde{f}^{(eq)} - \tilde{f}_0 - \varepsilon\tilde{f}_1 - \varepsilon^2\tilde{f}_2 - \dots)$$

$$\varepsilon^0: \tilde{f}^{(eq)} = +\tilde{f}_0$$

$$\varepsilon^1: \frac{\partial \tilde{f}_0}{\partial t} + \tilde{c}_\alpha \frac{\partial \tilde{f}_0}{\partial \tilde{x}_\alpha} = -\tilde{\nu}\tilde{f}_1$$

$$\varepsilon^k: \frac{\partial \tilde{f}_{k-1}}{\partial t} + \tilde{c}_\alpha \frac{\partial \tilde{f}_{k-1}}{\partial \tilde{x}_\alpha} = -\tilde{\nu}\tilde{f}_k$$

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BGK – eqn.

$$\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}}{\partial \tilde{x}_\alpha} = \frac{1}{\varepsilon} \cdot \tilde{\nu}\left(\tilde{f}^{(eq)} - \tilde{f}\right) \quad (1)$$ nondimensional form.

(non – dimensional form)

$$\varepsilon = K_n = \frac{\lambda}{L}$$ ← mean free path; ← char length scale.

Note:

$$\int_{\mathbb{R}^3} \phi(c)\,(f^{(eq)} - f)\, d\underline{c} = 0 \qquad \phi(c) = \begin{cases} m \\ mc \\ \frac{1}{2} m c^2 \end{cases}$$

→ e.g. $n = \int_{\mathbb{R}^3} f\, dc = \int_{\mathbb{R}^3} f^{(eq)}\, dc$

$n\underline{u} = \int_{\mathbb{R}^3} \underline{c} f\, dc = \int_{\mathbb{R}^3} c f^{(eq)}\, dc$

Perturbation around $f^{(eq)} \equiv f_0$

$$f = \sum_{k=0}^{\infty} \epsilon^k f_k$$

Substitute into BGK eqn:

$$\frac{\partial \tilde{f}_0}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}_0}{\partial \tilde{x}_\alpha} = -\tilde{\nu} \tilde{f}_1 \; : \epsilon_1 \quad (2)$$

$\vdots$

$$\frac{\partial \tilde{f}_k}{\partial \tilde{t}} + \tilde{c}_\alpha \frac{\partial \tilde{f}_k}{\partial \tilde{x}_\alpha} = -\tilde{\nu} \tilde{f}_{k+1} \; : \epsilon_{k+1} \; ; \; \epsilon \equiv \varepsilon \equiv K_n$$

Consider (2) in dimensional form:

$$\underbrace{\frac{\partial f_0}{\partial t} + c_\alpha \frac{\partial f_0}{\partial x_\alpha}}_{\frac{Df_0}{Dt}} = -\varepsilon \nu f_1 \quad (3)$$

$$\boxed{|c-u|^2 = \xi^2 = \xi_1^2 + \xi_2^2 + \xi_3^2}$$

Recall:

$$f_0 = \frac{n(x,t)}{(2\pi RT)^{3/2}} e^{\frac{-|c-u|^2}{2RT}} \qquad \left(f = n\hat{f}\right)$$

$$\frac{Df_0}{Dt} = \hat{f}_0 \frac{Dn}{Dt} + n \frac{D\hat{f}_0}{Dt}$$

$$= \hat{f}_0 \frac{Dn}{Dt} + n\left(\frac{\partial \hat{f}_0}{\partial T} \frac{DT}{Dt} + \frac{\partial \hat{f}_0}{\partial u_\alpha} \frac{Du_\alpha}{Dt}\right)$$

$$\frac{\partial \hat{f}}{\partial u_\alpha} = \hat{f}_0 \left(\frac{\xi^2}{2RT^2} - \frac{3}{2T}\right) = \hat{f}_0 \left(\frac{\xi^2}{2RT} - \frac{3}{2}\right) \frac{1}{T}$$

$$(3) \Rightarrow \varepsilon \upsilon f_1 = -\hat{f}_0 \left\{ \frac{Dn}{Dt} + n\left(\frac{\xi^2}{2RT} - \frac{3}{2}\right) \underbrace{\frac{1}{T}\frac{DT}{Dt}}_{\frac{D\ln T}{Dt}} + n\frac{\xi_\alpha}{RT}\frac{Du_\alpha}{Dt} \right\}$$

Consider Moment Relations:

$$(i)\ \frac{\partial n}{\partial t} + \frac{\partial(n u_\alpha)}{\partial x_\alpha} = 0$$

$$\Longleftrightarrow \frac{\partial n}{\partial t} + u_\alpha \frac{\partial n}{\partial x_\alpha} = -n\frac{\partial u_\alpha}{\partial x_\alpha}$$

$$(i)\ \frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_\alpha)}{\partial x_\alpha} = 0$$

$$(ii)\ \frac{\partial(\rho u_\alpha)}{\partial t} + \frac{\partial(\rho u_\alpha u_\beta)}{\partial x_\beta} + \frac{\partial P_{\alpha\beta}}{\partial x_\beta} = 0$$

$$(iii)\ \frac{\partial E}{\partial t} + \frac{\partial E u_\beta}{\partial x_\beta} + \frac{\partial P_{\alpha\beta} u_\beta}{\partial x_\beta} + \frac{\partial q_\beta}{\partial x_\beta} = 0$$

$$P_{\alpha\beta} = m\int_{\mathbb{R}^3} \xi_\alpha \xi_\beta f \, d\xi$$

$$(ii)\ \frac{\partial(n u_\alpha)}{\partial t} + \frac{\partial(n u_\alpha u_\beta)}{\partial x_\beta} + \frac{1}{m}\frac{\partial P_{\alpha\beta}}{\partial x_\beta} = 0$$

$$\Longleftrightarrow u_\alpha\left(\cancel{\frac{\partial n}{\partial t} + \frac{\partial n u_\beta}{\partial x_\beta}}\right) + n\left(\frac{\partial u_\alpha}{\partial t} + u_\beta\frac{\partial u_\alpha}{\partial x_\beta}\right)$$

$$+ \frac{1}{m}\frac{\partial}{\partial x_\beta}\underbrace{\int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \left(f_0\right.}_{P\delta_{\alpha\beta}} + \underbrace{\varepsilon f_1 + \dots}_{\text{higher-order term}}\left.\right) d\xi = 0$$

$$(iii)\ \frac{\partial T}{\partial t} + u_\beta \frac{\partial T}{\partial x_\beta} = -\frac{2}{3} T \frac{\partial u_\beta}{\partial x_\beta}$$

check!!

$$\Longleftrightarrow \frac{\partial \ln T}{\partial t} + u_\beta \frac{\partial \ln T}{\partial x_\beta} = -\frac{2}{3}\frac{\partial u_\beta}{\partial x_\beta}$$

$$\Longleftrightarrow \varepsilon \upsilon f_1 = -\hat{f}_0 \left\{ -n\frac{\partial u_\beta}{\partial x_\beta} + \xi_\beta \frac{\partial n}{\partial x_\beta} + n\left(\frac{\xi^2}{2RT} - \frac{3}{2}\right)\left(\xi_\beta \frac{\partial \ln T}{\partial x_\beta} - \frac{2}{3}\frac{\partial u_\beta}{\partial x_\beta}\right) \right.$$

$$\left. + n\frac{\xi_\alpha}{RT}\left(\xi_\beta \frac{\partial u_\alpha}{\partial x_\beta} - \frac{1}{\rho}\frac{\partial P}{\partial \alpha}\right) \right\}$$

$$= -\hat{f}_0 \left\{ \xi_\beta \frac{\partial n}{\partial x_\beta} + \underbrace{n\left(\frac{\xi^2}{2RT} - \frac{3}{2}\right)\xi_\beta \frac{\partial \ln T}{\partial x_\beta}}_{(a)} - n\frac{\xi^2}{3RT}\frac{\partial u_\beta}{\partial x_\beta} + n\frac{\xi_\alpha}{RT}\left(\xi\frac{\partial u_\alpha}{\partial x_\beta} - \frac{1}{\rho}\frac{\partial P}{\partial \alpha}\right) \right\}$$

(*)

Use ideal gas:

$$\frac{\partial n}{\partial x_\beta} = \frac{\partial}{\partial x_\beta}\left(\frac{P}{k_B T}\right)$$

$$= \frac{1}{k_B T}\frac{\partial P}{\partial x_\beta} - \frac{P}{k_B T^2}\frac{\partial T}{\partial x_\beta}$$

$$P = \rho R T = n k_B T \Rightarrow \frac{1}{k_B T} = \frac{n}{\rho R T}$$

$$= \underbrace{\frac{n}{\rho RT}\frac{\partial P}{\partial x_\beta}}_{(*)} - \underbrace{\frac{P}{k_B T}\frac{\partial \ln T}{\partial x_\beta}}_{(b)}$$

$= n$

(a)+(b)

$$\varepsilon \upsilon f_1 = -\hat{f}_0 \left\{ n\left(\frac{\xi^2}{2RT} - \frac{5}{2}\right)\xi_\beta \frac{\partial \ln T}{\partial x_\beta} + \frac{n}{RT}\left(\xi_\alpha \xi_\beta - \frac{1}{3}\delta_{\alpha\beta}\xi^2\right)\frac{\partial u_\alpha}{\partial x_\beta} \right\}$$

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Now let,

$$f = f_0 + \varepsilon f_1$$

$$P_{\alpha\beta} = m \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta (f_0 + \varepsilon f_1) d\xi$$

$$= p\,\delta_{\alpha\beta} - \frac{\rho}{\nu} \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \hat{f}_0 \left( \left(\frac{\xi^2}{2RT} - \frac{5}{2}\right) \xi_\gamma \frac{\partial \ln T}{\partial x_\gamma} + \frac{1}{RT}\left(\xi_\gamma \xi_\sigma - \frac{1}{3}\delta_{\gamma\sigma}\xi^2\right) \frac{\partial u_\gamma}{\partial x_\sigma} \right)$$

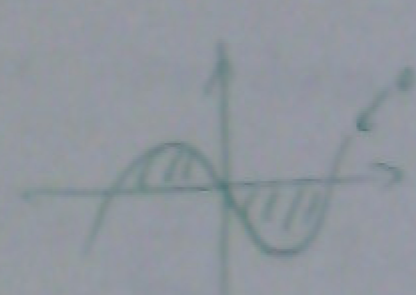
Consider:

$$\int_{\mathbb{R}^3} \xi_1^{l} \xi_2^{m} \xi_3^{n} \hat{f}_0 \, d\xi$$

→ permutations

$= 0$ if any $l, m, n$ is odd

due to symmetry, if function is odd $(\xi_1, \xi_2, \xi_3)$, integrates to zero!




Consider:

$\alpha \neq \beta$

$$P_{\alpha\beta} = \frac{-\rho}{\nu RT} \frac{\partial u_\gamma}{\partial x_\sigma} \int_{\mathbb{R}^3} \xi_\alpha \xi_\beta \xi_\gamma \xi_\sigma \hat{f}_0 \, d\xi$$

even only if $\alpha = \gamma$, $\beta = \sigma$ or $\alpha = \sigma$, $\beta = \gamma$

$$= \frac{-\rho}{\nu RT} \left( \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right) \underbrace{\int_{\mathbb{R}^3} \hat{f}_0 \xi_\alpha^2 \xi_\beta^2 \, d\xi}_{(RT)^2}$$

$$= \frac{-\rho RT}{\nu} \left( \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right)$$

Consider:

$\alpha = \beta$

$$P_{\alpha\beta} = p - \frac{\rho}{\nu RT} \int_{\mathbb{R}^3} \hat{f}_0 \xi_\alpha^2 \left( \xi_\gamma \xi_\sigma - \frac{1}{3}\delta_{\gamma\sigma}\xi^2 \right) \frac{\partial u_\gamma}{\partial x_\sigma} d\xi$$

$$= p - \frac{\rho RT}{\nu} \left( 2\frac{\partial u_\alpha}{\partial x_\alpha} - \frac{2}{3}\frac{\partial u_\beta}{\partial x_\beta} \right)$$

special case: no summation

$$P_{\alpha\beta} = p\,\delta_{\alpha\beta} - \frac{\rho}{\nu RT} \left( \frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} - \frac{2}{3}\delta_{\alpha\beta}\frac{\partial u_\gamma}{\partial x_\gamma} \right)$$

Heat flux

$$q_\beta = \frac{m}{2} \int_{\mathbb{R}^3} \xi_\beta \xi^2 (f_0 + \varepsilon f_1) d\xi = \underbrace{\frac{5}{2}R}_{c_p} \underbrace{\frac{p}{\nu}}_{\mu} \frac{\partial T}{\partial x_\beta}$$

Issues of BGK model

; if we set $\nu$ to properly recover viscosity, BGK enforces the heat conduction coefficient. these two are not independent of each other

also, $Pr = \frac{c_p \mu}{K} = 1$ for BGK model.

must know the steps! will be in exams!

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## Ch. 8. Lattice Gas Automata

So far: kinetic theory

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial x_\alpha} = \begin{cases} J(f,f) & \text{Boltzmann} \\ \frac{1}{\tau}(f^{(eq)} - f) & \text{BGK.} \end{cases}$$

$c = (c_\alpha)_{\alpha=1,2,3} \in \mathbb{R}^3$

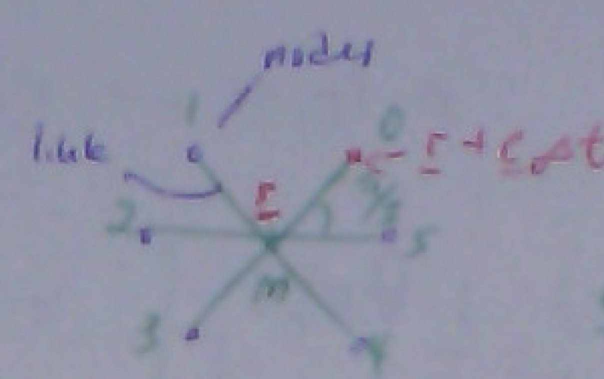

2D illustration $\underline{c} = \begin{pmatrix} c\cos\phi \\ c\sin\phi \end{pmatrix}$

$c \in [0, \infty)$

$\phi \in [0, 2\pi)$

## (8.1) lattice-gas Model

Idea: Restrict $|\underline{c}| = c$ to <u>one</u> value $c \equiv c_{ref}$ and <u>six</u> angles $\phi$




$\underline{c} = c(\cos(\frac{\pi}{3}k), \sin(\frac{\pi}{3}k))$,
$k = 0, \dots, 5$

Let $\Delta t$ be fixed. Assume, we simulate gas by taking "snapshots" at time instances $\Delta t\, n$; $n \in \mathbb{N}$

Assume non-dimensional variables:

$\tilde{c} = \frac{c}{c_{ref}} = 1$

$\tilde{m} = \frac{m}{m_{ref}}$

$\tilde{t} = \frac{t}{\Delta t} \Rightarrow \Delta\tilde{t} = 1$

$|c_\alpha| = 1$

## Simulate Lattice-gas

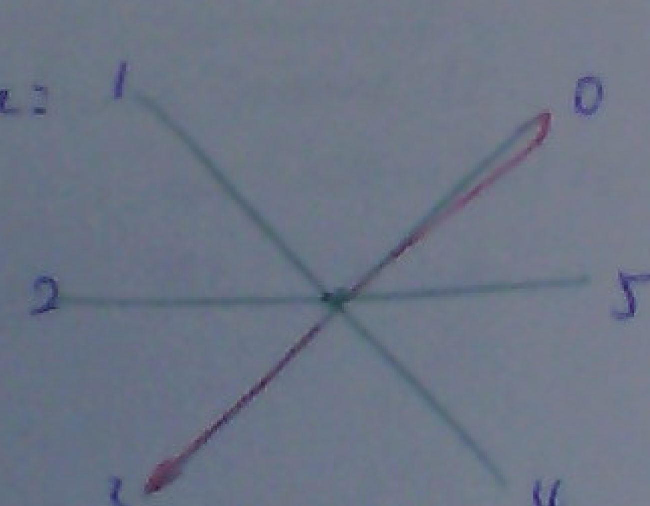
### Need Model:

1. "Lattice Configuration"

At each nodes $\underline{r}$ there can only be <u>one</u> particle having velocity $c_k$. $\boxed{\text{"exclusion principle"}}$

$\Rightarrow$ can encode the <u>state</u> at node $\underline{r}$ (at time $t$) using <u>6-bit</u> binary number.

Example:




node: 5 4 3 2 1 0

$\Rightarrow (0\,0\,1\,0\,0\,1) = n(\underline{r}, t)$

there are total of $2^6 = 64$ possible states at a given time.

## (ii) "Evolution"

Two-step operator.

"collision"  (0, 1) could be zero or 1 at node.

$$n_i'(\underline{r},t) = n_i(\underline{r},t) + \Delta_i(\underline{r},t) \quad ; i = 0, \dots, 5$$

"streaming"  recall, $\underline{c} = (\cos(\frac{\pi}{3}i), \sin(\frac{\pi}{3}i))\, c$  $=1$

$$n_i(\underline{r}+\underline{c}_i, t+1) = n_i'(\underline{r},t)$$

### Collision Model

Define: "collision" is a mapping $\Delta_i : \{0,1\} \to \{0,1\}$

$$n_i(\underline{r},t) \longmapsto n_i'(\underline{r},t)$$

need conservation

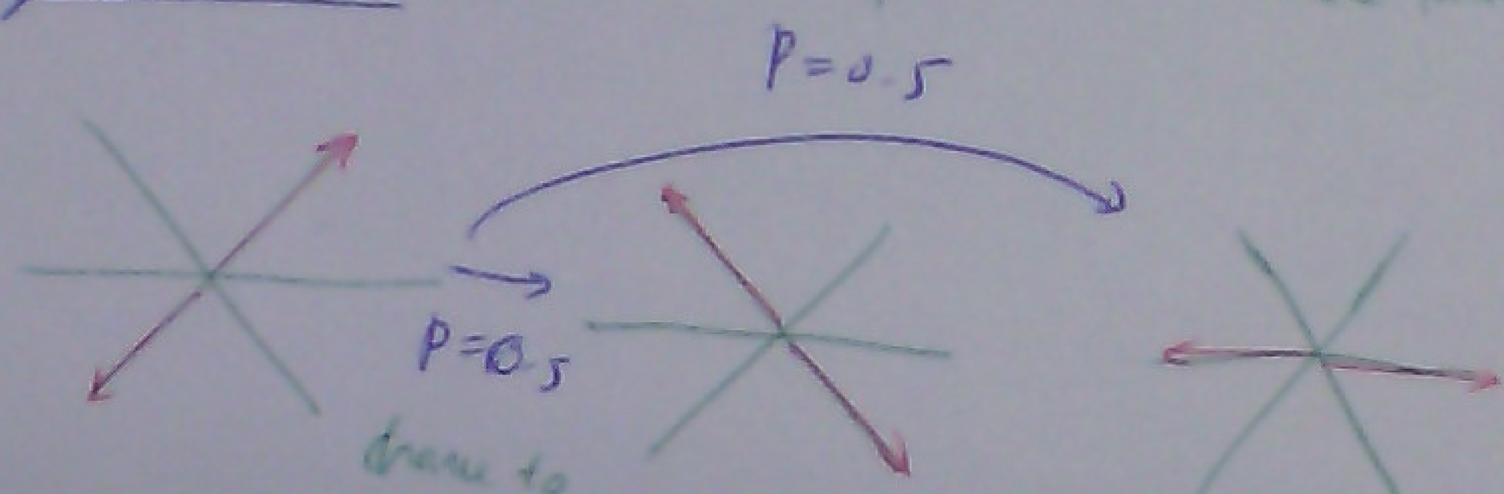
mass: $\sum_{i=0}^{5} n_i'(\underline{r},t) = \sum_{i=0}^{5} n_i(\underline{r},t) \quad ; \forall \underline{r}, t.$

momentum: $\sum_{i=0}^{5} n_i' c_i = \sum_{i=0}^{5} n_i c_i$

Energy: $\sum_{i=0}^{5} n_i c^2 = \sum_{i=0}^{5} n_i' c^2$  since there is only 1 possible $c$, (not $\underline{c}$) it holds from mass & momentum conservation, automatically.

### (i) Binary Collision

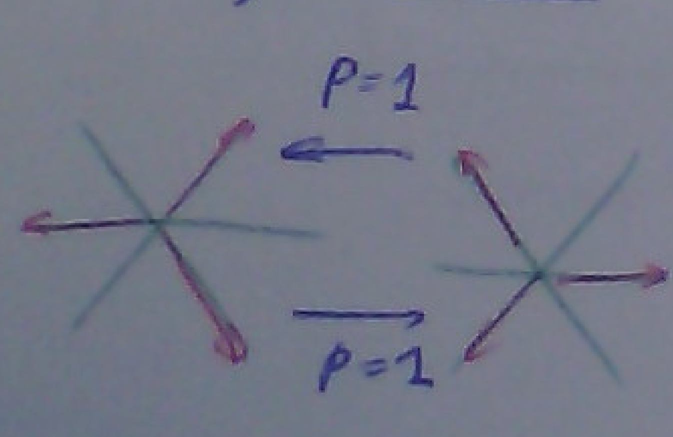
(each collision experienced at a node must conserve mass & momentum!)



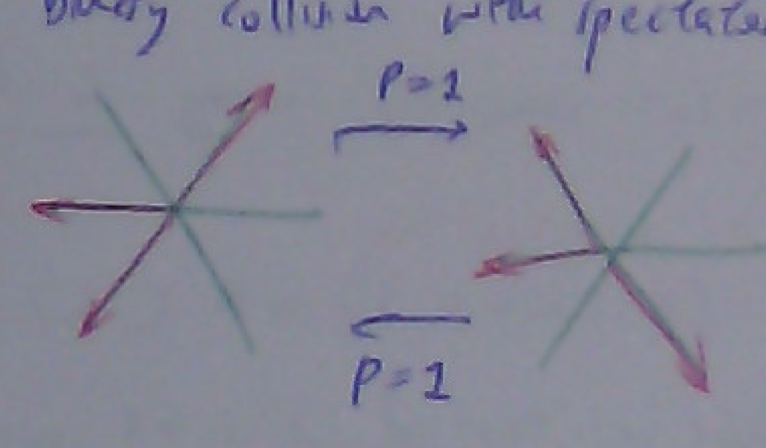

drawn to evolve to this state after collision, and vice-versa.

### (ii) three-way collision

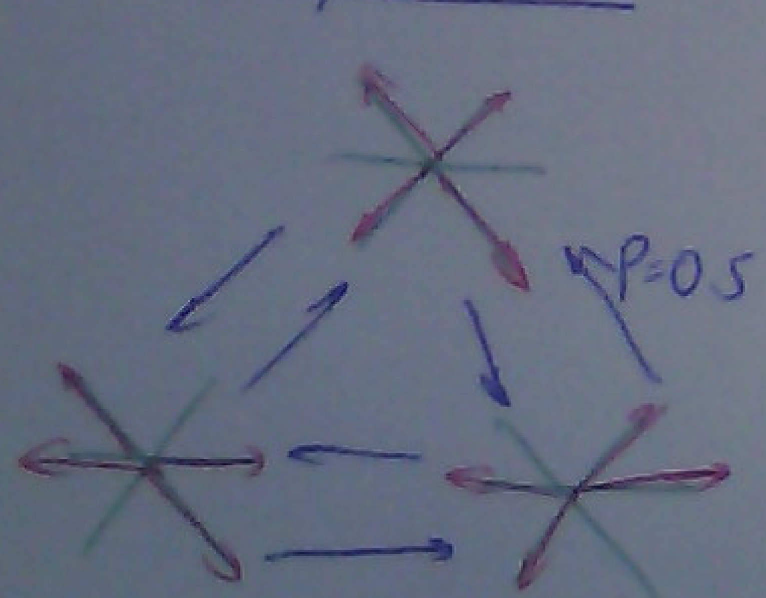
(a)




(b) "binary collision with spectator"




### (iii) Four-way collision




→ exclude trivial collision that is e.g. six-way collision.

→ in another words, if the configuration doesn't change, we don't consider it. (trivial collision)

## (8.3) Analysis of the LGA

### (8.3.1) The Collision Operator:

$$n_i'(\underline{r},t) = n_i(\underline{r},t) + \Delta_i(\underline{r},t) \quad ; \quad \Delta_i \in \{-1, 0, 1\}$$

Remark: In the following

$$\overline{i+k} = \begin{cases} i+k & \text{if } i+k < 6 \\ i+k-6 & \text{if } i+k \geq 6 \end{cases} \qquad i,k = 0, \dots, 5$$

essentially, this is a mod operator in C programming $\Rightarrow$ i % 6 + i=7, i=> 1.

Derive an algebraic Expression for $\Delta_i$

Then $\Delta = (\Delta_i)_{i=0,\dots,5}$

Consider Binary collision (Type (A))

| cases | $n_i$ | $n_{i+1}$ | $n_{i+2}$ | $n_{i+3}$ | $n_{i+4}$ | $n_{i+5}$ |
|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | 1 | 0 | 0 |
| 2 | 0 | 1 | 0 | 0 | 1 | 0 |
| 3 | 0 | 0 | 1 | 0 | 0 | 1 |

$$\delta_i^{(A,1)} = n_i n_{i+3} (1-n_{i+1})(1-n_{i+2})(1-n_{i+4})(1-n_{i+5})$$

$$\delta_i^{(A,2)} = n_{i+1} n_{i+4} (1-n_i)(1-n_{i+2})(1-n_{i+3})(1-n_{i+5})$$

$$\delta_i^{(A,3)} = \dots$$

Collision operator is constructed:

$$\Delta_i^{(A)} = a_1 \delta_i^{(A,1)} + a_2 \delta^{(A,2)} + a_3 \delta^{(A,3)}$$

$$a_1 = -1 \quad a_2 = \xi \; ; \; \xi = \{0, 1\} \quad a_3 = 1 - \xi.$$

"random bit"

$$\Rightarrow \Delta_i^{(A)} = -\delta_i^{(A,1)} + \xi \delta_i^{(A,2)} + (1-\xi)\delta_i^{(A,3)}$$

if initially case 1 of binary collision is detected, we know that after collision, $n_1$ will be zero definitely. Hence the $\Delta_i$ must be $-1$ at $n_1$.

Done similarly for 3-way collision:

$$\delta_i^{(B,1)} = n_i n_{i+2} n_{i+4} (1-n_{i+1})(1-n_{i+3})(1-n_{i+5})$$

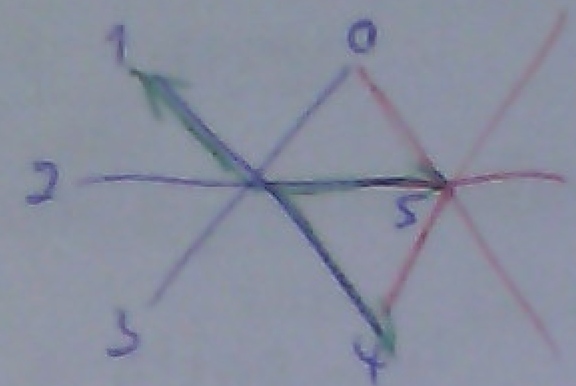
$$\delta_i^{(B,2)} = n_{i+1} n_{i+3} n_{i+5} (1-n_i)(1-n_{i+2})(1-n_{i+4})$$

$$\Delta_i^{(B)} = -\delta_i^{(B,1)} + \delta_i^{(B,2)}$$

$$\Rightarrow \Delta_i = \underbrace{A_i^{(A)} + \Delta_i^{(B)}}_{\text{allowed because it is a switch, either (A) is on or (B) is on.}}$$

## Implementation of LGA 1/12/2016

① preliminaries




$n = (110010)$

⊛ In practice: use 8 bit number

⊛ Possible datatypes

C: unsigned char
(int8_t (C99))

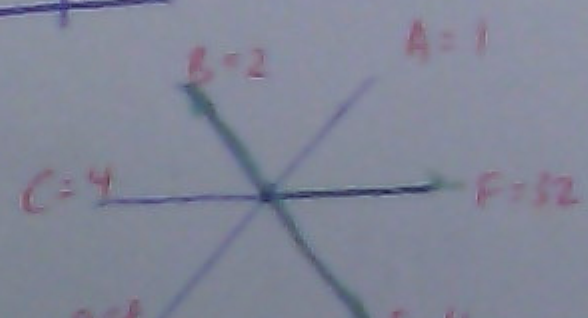
MATLAB: uint8

FORTRAN: INTEGER(1)
(90+)

### Algebraic vs. "Logical" method

i.e. Integer arithmetic or boolean operators.

**Example:**




$n = (110010)$ binary encoding → $A = (000001)_2$, $B = (000010)_2$, $C = (000100)_2$

$= 1 \cdot \underbrace{2^5}_{32} + 1 \cdot \underbrace{2^4}_{16} + 1 \cdot \underbrace{2^1}_{2}$

$= (50)_{10}$

Set state as

$n = B + E + F$
$= (50)_{10}$ } ① algebraic way

or: (in C programming)

bit shift operator: $(000001) \Rightarrow (000010)$

$n = \underbrace{(1 \ll 1)}_{B} \mid \underbrace{(1 \ll 4)}_{E} \overset{OR}{\mid} \underbrace{(1 \ll 5)}_{F};$

$\Rightarrow (000010) = B$
or $(010000) = E$
or $(100000) = F$

$(110010)_2 = (50)_{10}$

~~Ini~~

**Initialization**

Start with

$\frac{1}{6} \sum_{i=0}^{5} N_i =: \rho \quad \rho \in [0,1]$

average $\langle n_i \rangle$

① algebraic method

Set $\rho = \rho_0 \in [0,1]$ ; $n = (n_5, \dots n_0)$

$A = C_0$
$B = C_1$
$C = C_2$

```
for s = 1, ..., N_s        (# nodes)
    n = (r_s, t=0) = 0
    for k = 0, ..., 5
        if ⌊rand + ρ_0⌋        (=1, then populate; floor function: 1.2 => 1)
            n_k(r_s, t=0) += C_k
        end if
    end for
end for
```

① boolean method

bit 'OR'

$$\begin{array}{r} (001001) \\ (100000) \\ \hline (101001) \end{array}$$

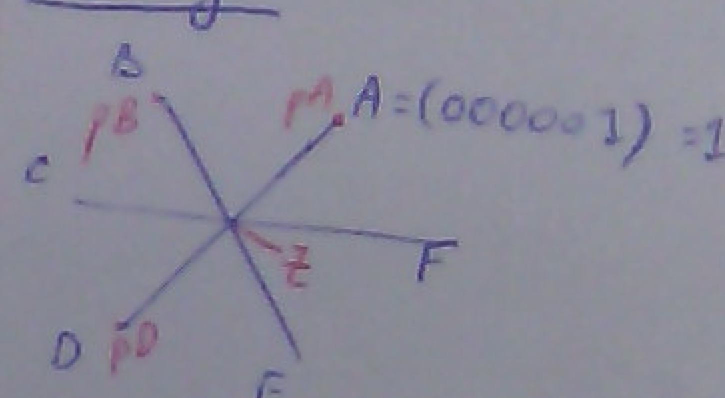
```
for s = 1, ..., N_s
    n(r_s, t=0) = 0
    for k = 0, ..., 5
        if ⌊rand + ρ_0⌋ (=1)
            n_k(r_s, t=0) |= (1 << k)
        end if
    end for
end for
```

**Collision:** implemented using lookup table.

| Index | | | value |
|---|---|---|---|
| B | $\xi$ | state (6 Bit) | |
| 0 | 0 | 000000 | (0 0) 000000 |
| 0 | 0 | 000001 | 000001 |
| 0 | 0 | 000010 | 000010 |
| | | ⋮ | ⋮ |
| 0 | 0 | 001001 | 010010 - 9th entry |
| | | ⋮ | ⋮ |
| | | 010101 | 101010 - 21st entry |
| | | ⋮ | |
| | | 111111 | 111111 - 63rd entry |
| 0 | 1 | 000000 | 000000 - 64th entry |
| ⋮ | | ⋮ | ⋮ |
| | 1 | 001001 | 100100 |
| | 1 | 111111 | 111111 |
| 1 | 0 | 000000 | |

B-bit is for boundary conditions.
$\xi$-bit is the random 1 ‖ 0.

**Streaming:**




Def: let ~~BA~~ pA be neighbour in "direction A"

$n(pA) \mathrel{|}= (n'(Z)\ \&\ A)$ ; $n'(Z)$ is state after collision. it checks whether particle occupies A after collision.

$n(pB) \mathrel{|}= (n'(Z)\ \&\ B)$

B=(0000 1 0)
n'=(010 1 1 0)

LBM 2nd Dec 2016 (1)

## LGA analysis

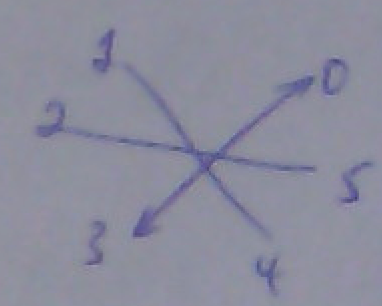
### The collision operator

~~$\Delta(n) = n_i' - n_i$ before collision~~

$$\Delta_i(n) = \overset{\text{after}}{n_i'(n)} - \overset{\text{before coll.}}{n_i}$$

$$n = (n_5\, n_4\, n_3\, n_2\, n_1\, n_0)$$

Recall:




$$n_0 n_3 (1-n_1)(1-n_2)(1-n_4)(1-n_5) = \begin{cases} 1 & \text{if } n = (001001) \\ 0 & \text{otherwise} \end{cases}$$

(001001)

Generalized Expression for identifying a state:

First, define set

$$S = \{0,1\}^6 = \{0,1\} \times \{0,1\} \times \{0,1\} \times \dots \times \{0,1\}$$
$$= \{(s_5, \dots, s_0) \,;\, s_i \in \{0,1\},\ i = 0, \dots, 5\} \qquad \#S = 64.$$

Now note: For $n_j, s_j \in \{0,1\}$

$$n_j^{s_j}(1-n_j)^{1-s_j} = \begin{cases} 1 & \text{if } n_j = s_j \\ 0 & \text{if } n_j \neq s_j \end{cases}$$

Check:

$$n_j = 0 = \begin{cases} s_j = 0 & : 0^0 \cdot 1^1 = 1 \\ s_j = 1 & : 0^1 \cdot 1^0 = 0 \end{cases}$$

Similar for $n_j = 1$.

⇒ Define "Algebraic" Kronecker Delta:

$$\delta_{n,s} = \prod_{j=0}^{5} n_j^{s_j}(1-n_j)^{1-s_j} = \begin{cases} 1, & n = s \\ 0, & n \neq s. \end{cases}$$

### Transition bit:

For each $s, s' \in S$ "transition bit"

$$\xi_{s,s'} = \begin{cases} 1 & s' \longleftrightarrow s \text{ connected by admissible collision } @ (r,t) \\ 0 & \text{otherwise} \end{cases}$$

Note: This will be set such that $\langle \xi_{s,s'} \rangle$ is the correct probability for transition between $s$ & $s'$.
expectation value of occurrence (probability)

Note:

$$\sum_{s' \in S} \langle \xi_{s,s'} \rangle = 1$$

$$\sum_{s' \in S} \xi_{s,s'} = 1$$ ; still 1 because at a given time, there can be only one result of transition

Function $\Delta_i(n) = n_i'(n) - n_i$

given input state $n$, output state is

$$n_i'(n) = \sum_{s \in S} \sum_{s' \in S} s_i' \xi_{s,s'} \underbrace{\prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j}}_{\delta_{n,s}}$$

only one for $s$ of the admissible transition

$$n_i = \sum_{s \in S} s_i \delta_{n,s}$$
$$= \sum_{s'} \sum_{s} s_i \delta_{n,s} \xi_{s,s'}$$

$$\Delta_i(n) = \sum_{s,s' \in S} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j}$$

| | Kinetic Theory | Lattice Methods |
|---|---|---|
| microdynamics | Eqn of motion for each particle. | LGA |
| Stochastic description | → Distribution function. $f(c,x,t)$<br>→ Equilibrium (maxwell-boltzmann) | |
| | For non equilibrium:<br>Boltzmann Equation. | "averaged" LGA<br>→ Lattice Boltzmann Method. |
| Conservation Laws | → Moments<br>+ Chapman-Enskog. | (discrete) Moments<br>+ Multiscale Expansion. check back on N-S eqn derivation. |

Equilibrium Solution of LGA

Postulate $N_i$: Probability of ~~the~~ link $i$ being occupied.
$P(n_i)=1$ ; $n_i = \int f \, dv$, taking discrete moments/prob.

Define: $\rho = \sum_{i=0}^{5} N_i$ $\quad \underline{u} = \frac{1}{\rho} \sum_{i=0}^{5} \underline{c}_i N_i$

statistically independent:
$N_i N_j$ : probability $P(n_i = 1 \; \& \; n_j = 1)$

1

LBM 8th

Recall:

Maxwell-

$f(s) =$

$\Rightarrow \frac{\partial f}{\partial t}$

$P(C \in$

con a

LGA

cc

(2

2

Consider:

$$P(n=(111111)) = \prod_{j=0}^{5} N_j$$

$$P(n=(000000)) = \prod_{j=0}^{5} (1-N_j)$$

$$P(n=(111000)) = \prod_{j=0}^{2} \overbrace{(1-N_j)}^{\text{prob of '0'}} \prod_{j=3}^{5} N_j$$

$$p(s) = \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$

$(s \in S)$

Assume $N_j$ is invariant under collision, hence conservation.

$$p(s') = \prod_{j=0}^{5} N_j^{s_j'} (1-N_j)^{1-s_j'}$$

carries information on allowed collision (transition from $s \to s'$.

$$= \sum_{s \in S} \langle \xi_{s,s'} \rangle \, p(s) \qquad \Sigma \text{ over 64 possible outcomes, } \{0,1\}.$$

$$= \sum_{s \in S} \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$

originally $s'$, but since it is a free index, can be renamed however it's liked.

$$\Rightarrow \sum_{s \in S} s_i \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j} = \sum_{s', s \in S} s_i' \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}$$

Since $\sum_{s' \in S} \langle \xi_{s,s'} \rangle = 1$. Multiply to LHS, then move the terms to LHS:

$$\sum_{s,s' \in S} (s_i' - s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j} = 0$$

$$\Rightarrow \underbrace{\prod_{j=0}^{5} (1-N_j)}_{\text{Assume } \neq 0} \underbrace{\left( \sum_{s,s' \in S} (s_i' - s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} \underbrace{\left( \frac{N_j}{1-N_j} \right)}_{\eta_j}^{s_j} \right)}_{=0} = 0$$

Multiply $\sum_{i=0}^{5} \log \eta_i$

$$\Rightarrow \sum_{i=0}^{5} \log \eta_i \sum_{s,s' \in S} (s_i' - s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} \eta_j^{s_j} = 0$$

$$= \sum_{s,s' \in S} \langle \xi_{s,s'} \rangle \left( \sum_{i=0}^{5} (s_i' - s_i) \log \eta_i \right) \prod_{j=0}^{5} \eta_j^{s_j} = 0$$

$$= \sum_{s,s' \in S} \langle \xi_{s,s'} \rangle \log \left( \frac{\prod \eta_i^{s_i'}}{\prod \eta_i^{s_i}} \right) \underbrace{\prod_{j=0}^{5} \eta_j^{s_j}}_{x_s} = 0$$

$$\Rightarrow \sum_{s,s' \in S} \langle \xi_{s,s'} \rangle \log \left( \frac{x_{s'}}{x_s} \right) x_s = 0 \qquad (1)$$

Note:

$$\sum_{s,s' \in S} x_s \langle \xi_{s,s'} \rangle = \sum_s x_s \underbrace{\sum_{s'} \langle \xi_{s,s'} \rangle}_{1}$$

$$= \sum_s x_s$$

$$= \sum_{s'} x_{s'} \underbrace{\sum_s \langle \xi_{s,s'} \rangle}_{\text{not necessarily true, but assumed } = 1.}$$

note the difference: $\sum_s \langle \xi_{s,s'} \rangle$ vs $\sum_{s'} \langle \xi_{s,s'} \rangle$

$$= \sum_{s,s'} x_{s'} \langle \xi_{s,s'} \rangle$$

$$\Rightarrow \sum_{s,s'} (x_s - x_{s'}) \langle \xi_{s,s'} \rangle = 0 \qquad (2)$$

$$-((1) + (2)) = 0$$

$$\sum_{s,s'} \underbrace{\left(-x_s \log\left(\frac{x_{s'}}{x_s}\right) + x_{s'} - x_s\right)}_{\geq 0} \underbrace{\langle \xi_{s,s'} \rangle}_{\geq 0} = 0 \qquad (*)$$

$$\Updownarrow$$

$$\int_{x_{s'}}^{x_s} \log\left(\frac{t}{x_{s'}}\right) dt \geq 0$$

---

Case (1) $\langle \xi_{s,s'} \rangle = 0$ transition is allowed!

Case (2) $\langle \xi_{s,s'} \rangle \neq 0$ transition allowed!

(i) $s = s' \Rightarrow 0$

(ii) $x_s = x_{s'}$ $(s' \neq s)$ (*) will have non-trivial zero solution!

$$\Rightarrow \prod_{i=0}^{5} \eta_i^{s_i} = \prod_{i=0}^{5} \eta_i^{s_i'}$$

take log: $\sum_{i=0}^{5} (s_i' - s_i) \log \eta_i = 0.$

satisfied if $\log \eta_i = -(a + \underline{b} \cdot \underline{c}_i)$

$$\Rightarrow \eta_i = e^{-(a + \underline{b} \cdot \underline{c}_i)} = \frac{N_i}{1 - N_i}$$

$$\rightarrow 1 - N_i = N_i e^{a + \underline{b} \cdot \underline{c}_i}$$

$$1 = N_i (1 + e^{a + \underline{b} \cdot \underline{c}_i})$$

$$N_i = \frac{1}{(1 + e^{a + \underline{b} \cdot \underline{c}_i})}$$

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Recall:

① 

Maxwell-Boltzmann

$$f(\underline{c}) = A e^{-\beta^2 |\underline{c}-\underline{\alpha}|^2}$$

$$\Rightarrow \left.\frac{\partial f}{\partial t}\right|_{collision} = 0$$

$$P(\underline{c} \in V_c) = \frac{1}{n}\int_{V_c} f(\underline{c})\, d\underline{c}$$

Use moments:

$$n = \int_{\mathbb{R}^3} f(c)\, dc$$

$$n\underline{u} = \int_{\mathbb{R}^3} \underline{c}\, f(c)\, dc$$

$$\frac{3}{2} n k_B T = \frac{m}{2}\int_{\mathbb{R}^3} \underbrace{|\underline{c}-\underline{u}|^2}_{\xi} f(c)\, dc$$

can express $A, \beta, \underline{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ as function of $n, T, u = (u_1, u_2, u_3)$

LGA

~~def A.N~~ $n_i(\underline{r} + \underline{c}_i, t+1) = n_i(\underline{r}, t) + \Delta_i(\underline{r}, t)$

admits an equilibrium s. th. $\langle \Delta_i \rangle = 0$

(1) $\langle n_i \rangle = N_i^{(eq)} = \frac{1}{1+e^{a+\underline{b}\cdot\underline{c}_i}}, \quad i = 0, \dots, 5.$

(2) $\rho = \sum_{i=0}^{5} N_i^{(eq)}$

(3) $\rho \underline{u} = \sum_{i=0}^{5} \underline{c}_i N_i^{(eq)}$

cannot express $a$, $\underline{b} = (b_1, b_2)$ as functions of $\rho, \underline{u} = (u_1, u_2)$

② Preliminary steps:

Let $\underline{u} = (u_\alpha)_{\alpha=1,2}$

set $a = a(\rho, \underline{u})$

$\underline{b} = \underline{b}(\rho, \underline{u})$

small velocity approximation

$$a(\rho, u) = \underbrace{a(\rho, 0)}_{a_0(\rho)} + \underbrace{\left.\frac{\partial a}{\partial u_\alpha}\right|_{(\rho,0)}}_{a_{1,\alpha}(\rho)} u_\alpha + \frac{1}{2} \underbrace{\left.\frac{\partial a}{\partial u_\alpha \partial u_\beta}\right|_{(\rho,0)}}_{a_{2,\alpha\beta}} u_\alpha u_\beta + \dots$$

$\Rightarrow a = a_0(\rho) + a_{1,\alpha} u_\alpha + a_{2,\alpha\beta} u_\alpha u_\beta + \dots$

$b_\alpha = b_{0,\alpha}(\rho) + b_{1,\alpha\beta} u_\beta + b_{2,\alpha\beta\gamma} u_\beta u_\gamma + \dots$

$\boxed{\text{Constraints:}}$ will shape the final $N_i^{(q)}$

① At $\underline{u} = 0 \Rightarrow N_i = \text{Const } \forall i$

$\Rightarrow b_{0,\alpha} = 0 \quad \alpha = 1,2$

② Symmetry: $N_i$ should be invariant under

(i) coordinate reflection

Let $x \mapsto -x$

$(u \mapsto -u \quad c_i \longrightarrow -c_i)$

$\Rightarrow a$ symmetric in $\underline{u}$,

$b$ antisymmetry in $\underline{u}$

$\left.\dfrac{1}{1+e^{a+\underline{b}\cdot c_i}}\right\}$ if this is invariant under reflection,

$a = -a$

$\underline{b}\cdot \underline{c}_i = \underline{b}\cdot(-\underline{c}_i)$ ; $\underline{c}_i$ is symmetric, $\underline{b}$ should be anti in to preserve $N_i$

$\Rightarrow a_{1,\alpha} = 0 \quad \alpha = 1,2$

$b_{2,\alpha\beta\gamma} = 0 \quad \alpha,\beta,\gamma = 1,2$

(ii) isotropy:

$b_{1,\alpha\beta} = b_1 \delta_{\alpha\beta}$

$a_{2,\alpha\beta} = a_2 \delta_{\alpha\beta}$

$\Rightarrow a = a_0(\rho) + a_2(\rho) u^2$

$b = b_{1,\alpha} u_\alpha$

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Substitute (1) ($N_i^{(eq)}$)   LBM 8th Dec 2016   3

$$N_i^{(eq)} = \frac{1}{1+e^{g_i(\rho,u)}} \quad ; \; g_i = a_0(\rho) + a_2(\rho)u^2 + b_1 \underbrace{u_\alpha c_{i\alpha}}_{\underline{u}\cdot c_i}$$

2 Expand ~~At~~ $N_i^{(eq)}$ in $\underline{u}$

$$N_i^{(eq)} = \underbrace{N_i^{(eq)}(\rho,0)}_{a} + \underbrace{\frac{\partial N_i^{(eq)}}{\partial u_\alpha}\Big|_{\underline{u}=0}}_{b} u_\alpha + \frac{1}{2}\underbrace{\frac{\partial^2 N_i^{(eq)}}{\partial u_\alpha \partial u_\beta}\Big|_{\underline{u}=0}}_{c} u_\alpha u_\beta + O(u^3)$$

(a) $N_i^{(eq)}(\rho,0) = \dfrac{1}{1+e^{g(\rho,0)}} = \dfrac{1}{1+e^{a_0}} = \dfrac{\rho}{6} =: d; \; \rho = \sum_{i=0}^{5} N_i^{(eq)}$

(b) $\underbrace{(N_i^{(eq)})'}_{i} \underbrace{\dfrac{\partial g_i}{\partial u_\alpha}}_{iii}$   $(N_i^{(eq)})' = \left(\dfrac{1}{1+e^x}\right)'\Big|_{x=a_0}$

not exception!

(c) $\underbrace{(N_i^{(eq)})''}_{ii} \dfrac{\partial g_i}{\partial u_\alpha}\dfrac{\partial g_i}{\partial u_\beta} + (N_i^{(eq)})' \underbrace{\dfrac{\partial g_i}{\partial u_\alpha \partial u_\beta}}_{iv}$

(i) $(N_i^{(eq)})'\Big|_{u=0} = \dfrac{-e^{a_0}}{(1+e^{a_0})^2} = -\dfrac{1-d}{d}d^2 = d(d-1)$

(ii) $(N_i^{(eq)})''\Big|_{u=0} = \dfrac{e^{a_0}(e^{a_0}-1)}{(1+e^{a_0})^3} = \dfrac{1-d}{d}\cdot\dfrac{1-2d}{d}d^3 = d(d-1)(2d-1)$

(iii) $\dfrac{\partial g_i}{\partial u_\alpha}\Big|_{u=0} = b_1 c_{i,\alpha}$

(iv) $\dfrac{\partial g_i}{\partial u_\alpha \partial u_\beta}\Big|_{u=0} = 2a_2 \delta_{\alpha\beta}$

$$N_i^{(eq)} = d + d(d-1)b_1 c_{i\alpha}u_\alpha + \frac{1}{2}\underbrace{d(d-1)(2d-1)b_1^2 c_{i\alpha}c_{i\beta}}\,\underbrace{u_\alpha u_\beta}$$
$$+\frac{1}{2}\underbrace{d(d-1)}2a_2\delta_{\alpha\beta}\,u_\alpha u_\beta$$

$$\Rightarrow N_i^{(eq)} = \underbrace{d}_{N_i^{(eq)}(\rho,0)} + \underbrace{d(d-1)b_1 c_{i,\alpha}}_{\frac{\partial N_i^{(eq)}}{\partial u_\alpha}}u_\alpha + \frac{1}{2}\underbrace{d(d-1)\{(2d-1)b_1^2 c_{i\alpha}c_{i\beta} + 2a_2\delta_{\alpha\beta}\}}_{\frac{\partial^2 N_i^{(eq)}}{\partial u_\alpha \partial u_\beta}}u_\alpha u_\beta.$$

$\Rightarrow$

$$\rho = \sum_{i=0}^{5} N_i^{(eq)}$$

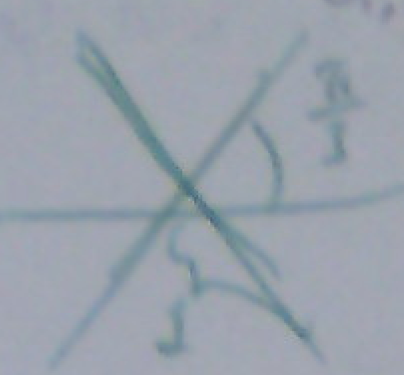
$$\rho \underline{u} = \sum_{i=0}^{5} \underline{c}_i N_i^{(eq)}$$

<u>Now:</u>

$$\sum_{i=0}^{5} c_{i,\alpha} = 0$$

$$\sum_{i=0}^{5} c_{i\alpha} c_{i\beta} = 3\delta_{\alpha\beta}$$

$$\sum_{i=0}^{5} c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$$




$c_{i,0} = \sin\left(\frac{\pi}{3}\right)$ or something similar

$c_{i,5} = \sin(0)$

(2)

$$\Rightarrow \rho = \sum N_i^{(eq)} = \overset{N_i^{(eq)}(\rho,0)}{\rho} + \frac{1}{2} d(d-1)\left\{12 a_2 \delta_{\alpha\beta} + 3(2d-1) b_1^2 \delta_{\alpha\beta}\right\} u_\alpha u_\beta$$

$$\Rightarrow a_2 = \frac{(1-2d)^3 b_1^2}{4} \Rightarrow a_2 = \frac{1-2d}{(d-1)^2}$$

(3)

$$\rho u_\beta = \sum \underline{c}_{i,\beta} N_i^{(eq)}$$

$$= d(d-1) b_1 \overbrace{\sum c_{i\alpha} c_{i\beta}}^{3\delta_{\alpha\beta}} u_\alpha = d(d-1) b_1 u_\beta \quad ; \quad \rho = 6d$$

$$\Rightarrow b_1 = \frac{2}{d-1}$$

$$\Rightarrow N_i^{(eq)} = d + 2d\, c_{i,\alpha} u_\alpha + \frac{d}{2(d-1)}\left\{2(1-2d)\delta_{\alpha\beta} + (2d-1)\, 4\, c_{i\alpha} c_{i\beta}\right\} u_\alpha u_\beta$$

$$= d + 2d(\underline{c}_i \cdot \underline{u}) + \underbrace{\frac{2d(2d-1)}{d-1}}_{\frac{\rho}{3}\underbrace{\left(\frac{2\rho-6}{\rho-6}\right)}_{G(\rho)}} \underbrace{\left(c_{i\alpha} c_{i\beta} - \frac{1}{2}\delta_{\alpha\beta}\right)}_{\underline{Q}_{\alpha\beta} \text{ (2nd order term)}} u_\alpha u_\beta$$

$$\boxed{N_i^{(eq)} = \rho\left\{\frac{1}{6} + \frac{\underline{c}_i \cdot \underline{u}}{3} + \frac{1}{3} G(\rho)\, Q_{\alpha\beta} u_\alpha u_\beta\right\}}$$

LGA equilibrium, accurate up to 2nd order (Taylor expansion)

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LGA: $n_i(\underline{r}+\underline{c}_i, t+1) = n_i'(\underline{r},t)$

$$n_i'(\underline{r},t) = n_i(\underline{r},t) + \Delta_i(\underline{r},t)$$

Conservation

$$\sum_{i=0}^{5} n_i' = \sum_{i=0}^{5} n_i \qquad N_i = \langle n_i \rangle \quad \left\{ \rho = \sum_{i=0}^{5} N_i \, , \, \rho\underline{u} = \sum_{i=0}^{5} \underline{c}_i N_i \right\}$$

$$\sum_{i=0}^{5} \underline{c}_i n_i' = \sum_{i=0}^{5} \underline{c}_i n_i \qquad (1) \sum_{i=0}^{5} \langle n_i \rangle = \sum_{i=0}^{5} N_i(\underline{r},t) = \sum_{i=0}^{5} N_i(\underline{r}+\underline{c}_i, t+1)$$

$$(2) \quad \& \sum \underline{c}_i N_i(\underline{r},t) = \sum \underline{c} N_i(\underline{r}+\underline{c}_i, t+1)$$

Multiscale expansion

Step 1: $N_i(\underline{r},t) = N_i^{(0)} + \varepsilon N_i^{(1)} + \varepsilon^2 N_i^{(2)} + \dots \quad \varepsilon = O(N^{-1})$ in Chapman-Enskog, $\varepsilon$ = knudsen number

$$N_i^{(eq)} = \frac{\rho}{6} + \frac{\rho}{3}(\underline{c}_i \cdot \underline{u}) + \frac{\rho}{3} G(\rho) Q_{i\alpha\beta} u_\alpha u_\beta$$

$$\boxed{G(\rho) = \frac{2\rho - 6}{\rho - 6} \; ; \; Q_{i\alpha\beta} = C_{i,\alpha} C_{i,\beta} - \frac{1}{2}\delta_{\alpha\beta}.} \approx \frac{1}{1+e^{a+b \cdot c_i}}$$

$$\sum N_i^{(eq)} = \rho \qquad \Rightarrow \qquad \sum_{i=0}^{5} N_i^{(k)} = 0 \qquad k = 1, 2, 3, \dots$$

$$\sum \underline{c}_i N_i^{(eq)} = \rho \underline{u} \qquad \qquad \sum_{i=0}^{5} \underline{c}_i N_i^{(k)} = 0$$

Step 2:

Three relevant time scales

$t = t^{(0)}$ "noise" - scale of micro-mechanics.

$t^{(1)} = \varepsilon t \; ; \; \varepsilon = O(N^{-1})$ "convection" - time scale for information to pass through domain.

$t^{(2)} = \varepsilon^2 t \; ;$ "diffusion"

multiscale modeling

$t^{(0)}$ = averaged out (over large time scale)

assume $g(t^{(1)}(t), t^{(2)}(t))$ ; $\frac{\partial}{\partial t} = \partial_t = \frac{\partial}{\partial t^{(1)}} \frac{\partial t^{(1)}}{\partial t} + \frac{\partial}{\partial t^{(2)}} \frac{\partial t^{(2)}}{\partial t}$

$$\frac{\partial}{\partial r_\alpha} = \partial r_\alpha = \varepsilon \, \partial r_\alpha^{(1)}$$

Step 3

Taylor expansion

$N_i(\underline{r}+\underline{c}_i, t+1)$, Want to use (1) (2)

$$\Rightarrow N_i(\underline{r}+\underline{c}_i, t+1) = \underbrace{N_i(\underline{r}, t)}_{\text{substitute with expansion: } N_i^{(0)} + \varepsilon N_i^{(1)} + \varepsilon^2 N_i^{(2)} + \dots} + \varepsilon \partial_{r_\alpha}^{(1)} N_i c_{i,\alpha} + \varepsilon \partial_t^{(1)} N_i + \varepsilon^2 \partial_t^{(2)} N_i + \text{higher order terms}$$

Take moments in (1) and collect terms.

$$\varepsilon^1: \partial_t^{(1)} \underbrace{\sum_{i=0}^{5} N_i}_{\rho} + \partial_{r_\alpha}^{(1)} \underbrace{\sum_{i=0}^{5} c_{i,\alpha} N_i}_{\rho u_\alpha} = 0$$

... if $\partial t^{(2)}$ is ignored; Now, this by itself is conservation law $\partial_t \rho + \partial_x \rho u = 0$.

End of Preview

## Problems with LGA

- ⊛ Noise problem - need to statistically trace microdynamics and average out the noise (expensive) lots of averaging over time steps.
- ⊛ inconsistency in momentum equation. - possibly existence of $G(\rho)$ term
- ⊛ Viscosity
- ⊛ complexity of collision operator $(2^6)$ → # links, 6 for our case.

## From ~~LBM~~ LGA to LBM

LGA $\quad n_i(\underline{r}_i + \underline{c}_i, t+1) = n_i(\underline{r}, t) + \Delta_i(\underline{r}, t)$

$$\Delta_i = \sum_{s,s' \in S} (s_i' - s_i) \underbrace{\xi_{s,s'}}_{\text{transition bit}} \underbrace{\prod_{j=0}^{5} n_j^{s_j} (1-n_j)^{1-s_j}}_{d_{n,s}} \qquad (3)$$

**Step 1** Averaging the LGA

$$\langle n_i(\underline{r}+\underline{c}_i, t+1) \rangle = \langle n_i(\underline{r}, t) \rangle + \langle \Delta_i(\underline{r}, t) \rangle$$

$$N_i(\underline{r}+\underline{c}_i, t+1) = N_i(\underline{r}, t) + \langle \Delta_i(\underline{r}, t) \rangle$$

Split $n_i = \underbrace{\langle n_i \rangle}_{N_i} + \hat{n}_i$ ← fluctuation

$\Rightarrow \langle \hat{n}_i \rangle = 0$

$\langle N_i \rangle = N_i$

Substitute into (3)

$$\langle \Delta_i \rangle = \left\langle \sum_{s,s' \in S} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} (N_j + \hat{n}_j)^{s_j} (1 - N_j - \hat{n}_j)^{1-s_j} \right\rangle$$

$\langle N_i \hat{n}_j \rangle = N_i \langle \hat{n}_j \rangle = N_i \cdot 0 = 0$

Now: get items like $\langle (N_i + \hat{n}_i)(N_j + \hat{n}_j) \rangle = N_i N_j + \cancel{\langle N_i \hat{n}_j \rangle}^{0} + \cancel{\langle N_j \hat{n}_i \rangle}^{0} + \langle \hat{n}_i \hat{n}_j \rangle$

higher order terms, choose to neglect.

$$\Rightarrow N_i(\underline{r}+\underline{c}_i, t+1) = N_i(\underline{r}, t) + \underbrace{\sum_{s,s' \in S} (s_i' - s_i) \xi_{s,s'} \prod_{j=0}^{5} N_j^{s_j} (1-N_j)^{1-s_j}}_{C_i(N_i)}$$

$C_i(N_i^{(eq)}) = 0$, $N = (N_0, \dots, N_5)$

Summary:

- ⊕ Noise removed.
- ⊖ now susceptible to round-off errors.
- ⊖ increased storage requirements. 6 bit binary → 6 × 8 bit floating numbers
- ⊖ everything else, notably complexity $(2^6)$ flops.

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**Step 2** Linearizing collision operator

Denote

$$N_i^{(eq,0)} = N_i^{(eq)}\Big|_{\underline{u}=0}$$

Linearize around $\boxed{N_i^{(eq,0)}}$

$$(4)\quad C_i(N) = \cancel{C_i(N^{(eq)},0)}\ C_i(N^{(eq,0)}) + \frac{\partial C_i}{\partial N_j}\Big|_{\underline{u}=0}(N_j - N_j^{(eq)}) + \frac{1}{2}\frac{\partial^2 C_i}{\partial N_j \partial N_k}(N_j - N_j^{(eq,0)})(N_k - N_k^{(eq,0)})$$

+ higher-order terms.

collision op. → 0 with $N^{(eq)}$

$$(5)\quad 0 = C(N^{(eq)}) = C_i(N^{(eq,0)}) + \frac{\partial C_i}{\partial N_j}\Big|_{\underline{u}=0}(N_j^{(eq)} - N_j^{(eq,0)}) + \frac{1}{2}\frac{\partial^2 C_i}{\partial N_j \partial N_k}(N_j^{(eq)} \cdots) + \cdots$$

(4) − (5)

$$C_i \approx \frac{\partial C_i}{\partial N_j}(N_j - N_j^{(eq)}) + \text{higher order terms.}$$

→ neglecting.

$$\frac{\partial C_i}{\partial N_j} = \begin{pmatrix} \frac{\partial C_0}{\partial N_0} & \cdots & \frac{\partial C_0}{\partial N_5} \\ & & \\ \frac{\partial C_5}{\partial N_0} & & \frac{\partial C_5}{\partial N_5} \end{pmatrix}$$ 6×6 mat.

$$\Rightarrow N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + \left(\frac{\partial C_i}{\partial N_j}\right)(N_j - N_j^{(eq)})$$

Fermi-Dirac distribution (equilibrium)

moving towards to LBM, attempt to remove fermi-dirac dist. replace with Boltzmann dist.

**Note:** ⊕ Complexity now $b^2$ (before: $2^b$)

⊖ rest as before.

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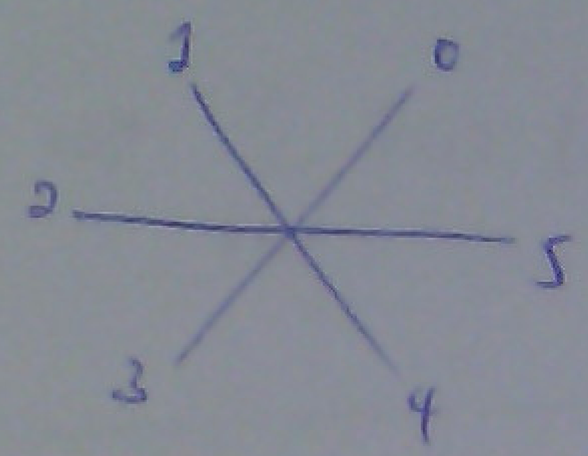
H - theorem for LGA




$n = (n_i)_{i=0,\dots,5}$

$= \cancel{(n_1\, n_2\, n_3\, n_4\, n_5\, n_6)}$

$= (n_5\, n_4\, n_3\, n_2\, n_1\, n_0)$

where $n_i = \{0,1\}$

$N_i = \langle n_i \rangle \equiv P(n_i = 1)$ — Probability of $n_i$ occupied

$1 - N_i \equiv P(n_i = 0)$ — $n_i$ not occupied

Equilibrium

$$\underset{\substack{\uparrow \\ s = \{0,1\}^6 = \{(s_5 \dots s_0) : s_i \in \{0,1\}\}}}{P(s \in S)} = \prod_{j=0}^{5} N_j^{s_j} (1 - \underset{\equiv N^{(eq)}}{N_j})^{1-s_j} \quad (1)$$

this comes as a consequence of $N_i \equiv N^{(eq)}$ $\Rightarrow P(s = (111000)) = N_5 N_4 N_3 (1 - N_2)(1 - N_1)(1 - N_0)$

---

Let $P(s)$ be general Probability of state $s \in S$, not necessarily (1)

$$\left( \sum_{s \in S} P(s) = 1 \right)$$

$$N_i = \cancel{\sum_{s \in S_i}} \sum_{s \in S} s_i P(s)$$

$$1 - N_i = \sum_{s \in S} (1 - s_i) P(s)$$

Now, Probability of $s' \in S$ after collision. (time $t'$)

$$\underbrace{P'(s')}_{P(s;\, x,\, t')} = \sum_{s \in S} \langle \xi_{s,s'} \rangle \underbrace{P(s)}_{P(s;\, x,\, t)}$$

we had — sum of all possible allowed collision states

$$\sum_{s' \in S} \langle \xi_{s,s'} \rangle = 1 \quad (2)$$

$$\sum_{s \in S} \langle \xi_{s,s'} \rangle = 1 \quad (3)$$

Proposition:

For any convex function $f$,

$$\sum_{s'} f(P'(s')) \leq \sum_{s} f(P(s))$$


proof:

Note $f$ convex $\Rightarrow f(\xi x_1 + (1-\xi) x_2) < \xi f(x_1) + (1-\xi) f(x_2) \quad ; \ \xi \in [0,1]$

Also holds for convex combination of n variables:

$$f\left(\sum_{j=1}^{n} \xi_j x_j\right) \le \sum_{j=1}^{n} \xi_j f(x_j) \quad ; \quad \sum_{j=1}^{n} \xi_j = 1$$ ← convex combination sums to 1.

$$\Rightarrow f\Big(\underbrace{\overbrace{\sum_{s\in S} \langle \xi_{s,s'}\rangle}^{=1\text{, from (2)}} P(s)}_{P(s')}\Big) \le \sum_{s\in S} \langle \xi_{s,s'}\rangle f(P(s))$$

Sum over all $s' \in S$:

$$\sum_{s'\in S} f(P'(s')) \le \sum_{s\in S} \underbrace{\sum_{s'\in S} \langle \xi_{s,s'}\rangle}_{=1} f(P(s))$$

$$= \sum_{s\in S} f(P(s)) \quad \blacksquare$$

$f = x \ln x$

$$\sum_{s'} P'(s') \ln P'(s') \le \underbrace{\sum_{s} P(s) \ln P(s)}_{H(S,t)}$$

Proposition

$$\sum_{s\in S^*} P(s) \ln P(s) \ge \underbrace{\sum_{i=0}^{S} N_i \ln N_i + (1-N_i)\ln(1-N_i)}_{(*)}$$

with equality iff:

$$P(s) = \prod_{j=0}^{S} N_i^{s_i}(1-N_i)^{1-s_i}$$

$s_1 \ln(N_1) + s_2 \ln(N_2) = \ln(N_1^{s_1}) + \ln(N_2^{s_2}) = \ln\left(\prod_{i=1}^{2} N_i^{s_i}\right)$

proof:

$$N_i = \sum_{s\in S} s_i P(s)$$

$$1 - N_i = \sum_{s\in S} (1-s_i) P(s)$$

$$(*) = \sum_{i=0}^{S}\left(\sum_{s\in S} s_i P(s) \ln(N_i) + \sum_{s\in S} (1-s_i) P(s) \ln(1-N_i)\right)$$

$$= \sum_{s\in S} P(s) \left(\sum_{i=0}^{S} \left(s_i \ln(N_i) + (1-s_i)\ln(1-N_i)\right)\right)$$

$$= \sum_{s\in S} P(s)\left(\ln\left(\prod_{i=0}^{S} N_i^{s_i}\right) + \ln\left(\prod_{i=0}^{S}(1-N_i)^{1-s_i}\right)\right) = \sum_{s\in S} P(s) \ln\left(\prod_{i=0}^{S} N_i^{s_i}(1-N_i)^{1-s_i}\right)$$

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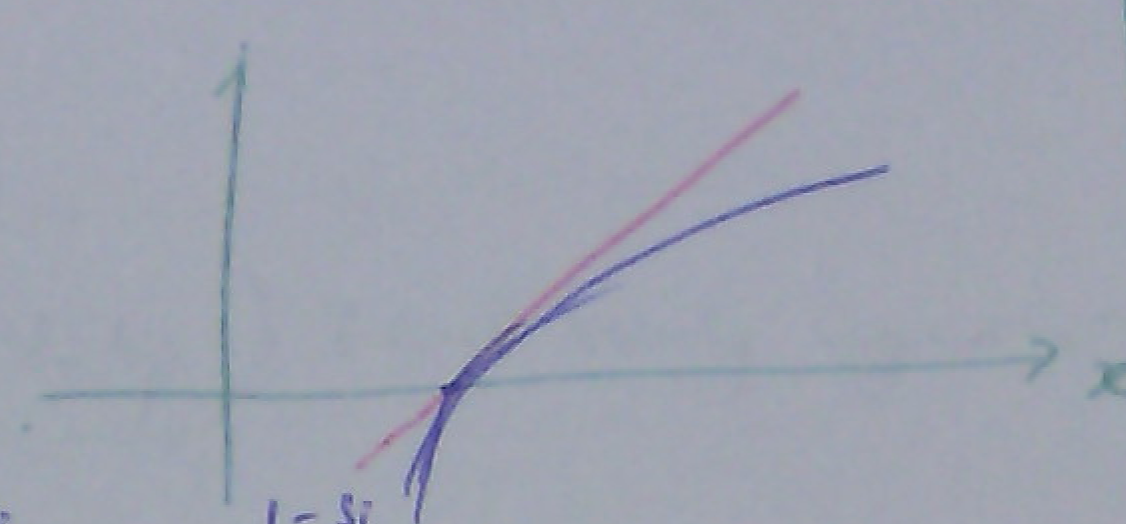
$$\overset{(4)}{\Rightarrow} \sum_{s \in \mathcal{S}} P(s) \ln P(s) \geq \sum_{s \in \mathcal{S}} P(s) \ln \left( \prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i} \right)$$

$$\Rightarrow \sum_{s \in \mathcal{S}} P(s) \ln \left( \frac{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}{P(s)} \right) \leq 0 \quad ☆$$

Note: get equality ~~at~~ iff

$$(5) \qquad P(s) = \prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}$$




otherwise, using $\ln x < x - 1 \quad (x \neq 1)$

$$\Rightarrow \ln \left( \frac{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}{P(s)} \right) < \frac{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}{P(s)} - 1$$

$$\sum_{s \in \mathcal{S}} P(s) \ln \left( \cdots \right) < \sum_{s \in \mathcal{S}} \cancel{P(s)} \left( \prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i} - P(s) \right)$$

misleading! (5) doesn't hold! , I compared to ☆

$$\text{r.h.s.} = \sum_{s \in \mathcal{S}} \Big( \underbrace{\prod_{i=0}^{5} N_i^{s_i} (1-N_i)^{1-s_i}}_{P^{(eq)}(s)} \Big) - 1$$

$= 0$

r.H.s becomes $= 0$ if (5) is used. otherwise, it is strictly less than 0.

$P^{(eq)}(s) \ni s = (1\ 1\ 1\ 1\ 1\ 1)$

$\to N_0 N_1 N_2 N_3 N_4 N_5$

$$\sum_{s \in \mathcal{S}} P^{(eq)}(s) = N_0 N_1 N_2 N_3 N_4 N_5 + N_0 N_1 N_2 N_3 N_4 (1-N_5) + N_0 N_1 N_2 N_3 (1-N_4) N_5 + N_0 N_1 N_2 N_3 (1-N_4)(1-N_5)$$

$= 1$

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②

LGA: Equilibrium

$$N_i^{(eq)} = \frac{1}{1 + e^{a + \underline{b} \cdot \underline{c}_i}} \quad (\text{"Fermi - Dirac"})$$

work at $a, \underline{b}$ as functions of

$\rho \; (= \sum_i N_i)$

$\underline{u} = (= \frac{1}{\rho} \sum_i \underline{c}_i N_i)$

$$N_i^{(eq)} \approx \rho \left( \frac{1}{6} + \frac{1}{3} \underbrace{c_{i\alpha} u_\alpha}_{\underline{c}_i \cdot \underline{u}} + G(\rho) \underbrace{Q_{i,\alpha\beta} u_\alpha u_\beta}_{(\underline{c}_i \cdot \underline{u})^2 - \frac{1}{2} u^2} \right) \quad (\text{small velocity approximation})$$

$$G(\rho) = \frac{1}{3} \cdot \frac{6 - 2\rho}{6 - \rho}$$ problematic

destroys consistency with NS.

$$Q_{i,\alpha\beta} = c_{i,\alpha} c_{i,\beta} - \frac{1}{2} \delta_{\alpha\beta}$$

$\boxed{\text{LGA to LBM}}$

Step 1 averaged LGA

$$N_i(\underline{r}_i + \underline{c}_i, t+1) = N_i(\underline{r}, t) + C_i(N), \quad N = (N_i)_{i=0,\dots,5}$$

$$C_i(N) = \sum_{s, s' \in S} (s_i' - s_i) \langle \xi_{s,s'} \rangle \prod_{j=0}^{5} N_j^{s_j} (1 - N_j)^{1 - s_j}$$

LGA is derived in attempt to bridge micro mechanics to macro scale dynamics (NS). clear, there are terms that is not consistent to NS. LBM will sever the ties with the problematic terms.

$$\boxed{\text{Note: } C_i(N_i^{(eq)}) = 0 \Rightarrow \sum_{i=0}^{5} C_i = 0, \quad \sum_{i=0}^{5} c_i C_i = 0}$$

Step 2. Linearize

$$\left. \frac{\partial C_i}{\partial N_j} \right|_{N^{(eq)}(\rho, u=0)} \quad (\text{matrix})$$

$$N_i(\underline{r} + \underline{c}_i, t+1) = N_i(\underline{r}, t) + \underbrace{\sum_{j=0}^{5} C_{ij}^{(0)} (N_j - N_j^{(eq)})}_{C_i(N)}$$

Note: $C[N_i^{(eq)}] \Rightarrow \sum_{i=0}^{5} C_i = 0, \quad \sum_{i=0}^{5} \underline{c}_i C_i = 0$

Step 3 "Model with enhanced collisions".

ⓐ in $N_i^{(eq)}$, we set $g(\rho) = \frac{1}{3} \cdot \boxed{\cancel{\frac{6-2\rho}{6-\rho}}} = 1$

$$\Rightarrow f_i^{(eq)} = \rho \left\{ \frac{1}{6} + \frac{1}{3} c_{i,\alpha} u_\alpha + \frac{1}{3} Q_{i,\alpha\beta} u_{\alpha\beta} \right\}$$

$$= \rho \left\{ \frac{1}{6} + \frac{1}{3} \underline{c}_i \cdot \underline{u} - \frac{u^2}{6} + \frac{1}{3} (\underline{c}_i \cdot \underline{u})^2 \right\}$$

Consider MB-distribution

$$f^{(MB)} = \frac{\rho}{(2\pi RT)} e^{\frac{-(c-u)^2}{2RT}}$$ for 2D case, in 3D, $\frac{\rho}{(2\pi RT)^{3/2}} \cdots$

$$= \boxed{\frac{\rho}{2\pi RT} e^{\frac{-c^2}{2RT}}}^{=A} \underbrace{e^{\frac{u \cdot c}{RT}} e^{-\frac{u^2}{2RT}}}_{*}$$

Note: $e^x = 1 + x + \frac{1}{2}x^2 + \ldots$

$$\Rightarrow * = 1 + \frac{u \cdot c}{RT} - \frac{u^2}{2RT} + \frac{(c \cdot u)^2}{(RT)^2} + O(u^3)$$

$\boxed{A = \frac{\rho}{6} \quad RT = \frac{1}{2}}$, matches $f_i^{(eq)}$ ~~...~~

(b) Replace $C_{ij}^{(0)}$ with

Matrix $A = (a_{ij})_{ij} = 1, \ldots, b$

satisfying conservation. $\to$ $\sum G_i = 0$, $\sum c_i G_i = 0$ ; $C_i = \sum_j a_{ij}(f_j - f_j^{(eq)})$

---

Lattice-Boltzmann Method.

$A_{ij} = -w\,\delta_{ij}$

$$f(r + c_i, t+1) = f_i(r,t) + \overbrace{w\left(f^{(eq)}(r,t) - f_i(r,t)\right)}^{C_i\text{, collision operator}}$$

$\rho = \sum f_i \stackrel{!}{=} \sum f_i^{(eq)}$

$\rho u = \sum c_i f_i \stackrel{!}{=} \sum c_i f_i^{(eq)}$

$\Rightarrow$ $\sum G_i = \sum f_i - f_i^{(eq)} = 0$

$\sum c_i G_i = \sum c_i(f_i - f_i^{(eq)}) = 0$

---

Remark:

Algorithm

Set $f(r, t=0)$ $\forall r$

do $n = 1, 2, 3, \ldots$

$\rho = \sum f_i \quad \rho u = \sum c_i f_i$

$f_i^{(eq)} = f_i^{(eq)}(\rho, u)$

$f_i' = w(f_i^{(eq)} - f_i)$ collision

$\forall r$ (locally)

$f(r + c_i, t+1) = f_i(r,t) + f_i'$ streaming

end do

etc b.c.

$$f_i^{(eq)} = \rho w_i \left(1 + \frac{c_i u}{c_s^2} - \frac{u^2}{2c_s^2} + \frac{1}{2}\frac{(c_i \cdot u)^2}{c_s^4}\right) ; c_s^2 = RT$$

## Computation of $w_i$

Review: Quadrature

$$I(f) = \int_a^b f \, dx \approx \sum_{i=1}^{n} \underbrace{\alpha_i}_{\text{weights}} \underbrace{f(x_i)}_{\text{nodes}} = I_n(f)$$

**Def:** (degree of precision d.o.p)

We say $I_n(f)$ has d.o.p $m \in \mathbb{N}$ if $I(x^l) - I_n(x^l) = 0 \quad \forall l \le m = 0, \dots, m.$

optimal quadrature rule:

gaussian $m = 2n - 1$.

Weighted Integrals

$$I^{(w)}(f) = \int_{a(-\infty)}^{b(\infty)} \underbrace{w(x)}_{\ge 0} f(x) \, dx = \sum_{i=1}^{n} \alpha_i f(x_i) = I_n^{(w)}(f)$$

Still:

$$I^{(w)}(x^l) - I_n^{(w)}(x^l) = 0 \quad \text{for gaussian rule}, \; l = 0, \dots, 2n-1$$

---

Example: $b = \infty$, $a = -\infty$

$w(x) = e^{-x^2}$

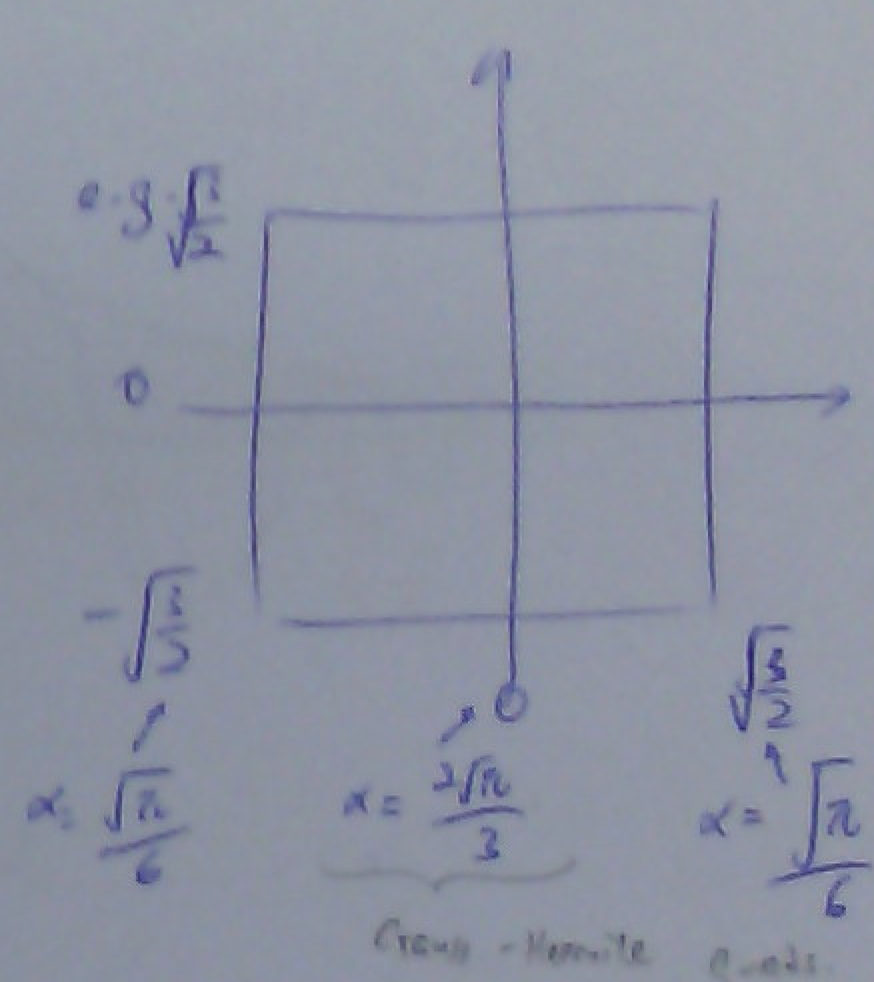
$\Rightarrow$ gauss - Hermite quadrature

---

Multivariate case

$$I^{(w)}(f) = \int_{\mathbb{R}^2} e^{-|x|^2} f(x) \, dx \, dy \; ; \; |x|^2 = x^2 + y^2$$

$$\approx \sum_{i,j=1}^{n} \underbrace{\alpha_i \beta_j}_{\text{weights, as in 1D}} f(x_i, y_j)$$




Recall:

$$\circledast \; f^{(eq)}_{MB} = \underbrace{\frac{\rho}{2\pi RT} e^{-\frac{c^2}{2RT}}}_{A} \left( 1 + \frac{c \cdot u}{RT} - \frac{u^2}{2RT} + \frac{1}{2} \cdot \frac{(c \cdot u)^2}{(RT)^2} \right)$$

$$\int_{\mathbb{R}^2} f^{(eq)} \, dc = \rho$$

$$\int_{\mathbb{R}^2} f^{(eq)} \, dc = \rho \underline{u}$$

Want:

$$\sum_{i=0}^{1} f_i^{(eq)} = \rho$$

$$\sum \underline{c}_i f_i^{(eq)} = \rho \underline{u}$$

and possibly higher-order moments (same as from M-B)

Consider:

$$I = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^n c_2^m \, d\underline{c} \quad ; \quad \tilde{f}^{(eq)} \text{ as in } *$$

replace with Gauss-Hermite quadrature.

Multiscale Expansion

Consider ODE:

$$y(t) = a\sin(t) + b\cos(t)$$

$$y'(t) = a\cos(t) - b\sin(t)$$

$$y''(t) = -a\sin(t) - b\cos(t)$$

(i) $y'' + y = 0 \Rightarrow y(t) = a\cos(t) + b\sin(t)$

$y(0) = 0 \qquad y(0) = 0 = a$

$y'(0) = 1 \qquad y'(0) = -b = 1$

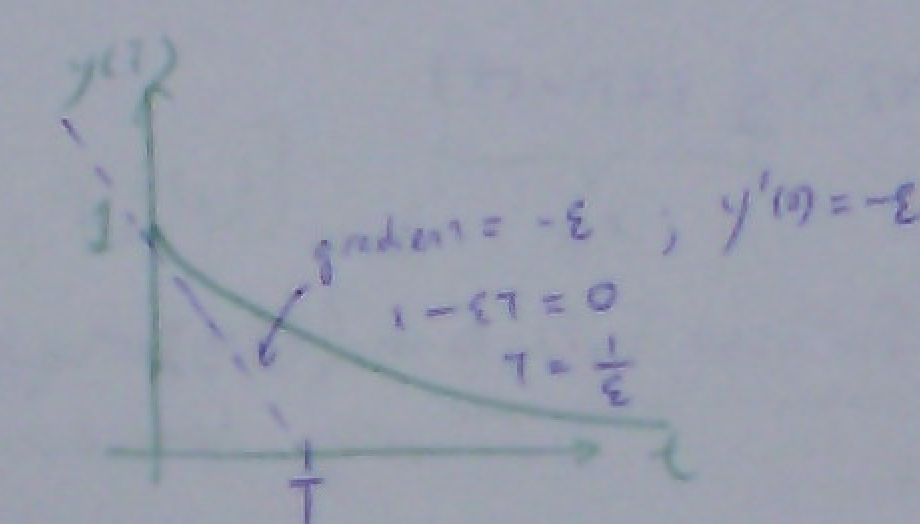
$\Rightarrow y(t) = b\sin(t) = -1\sin(t)$

Relevant time scale: $T = 2\pi = \mathcal{O}(1)$

(ii) $y' + \varepsilon y = 0 \Rightarrow y(t) = a e^{-\varepsilon t}$

$y(0) = 1 \qquad y(0) = a = 1$

$y(t) = e^{-\varepsilon t}$



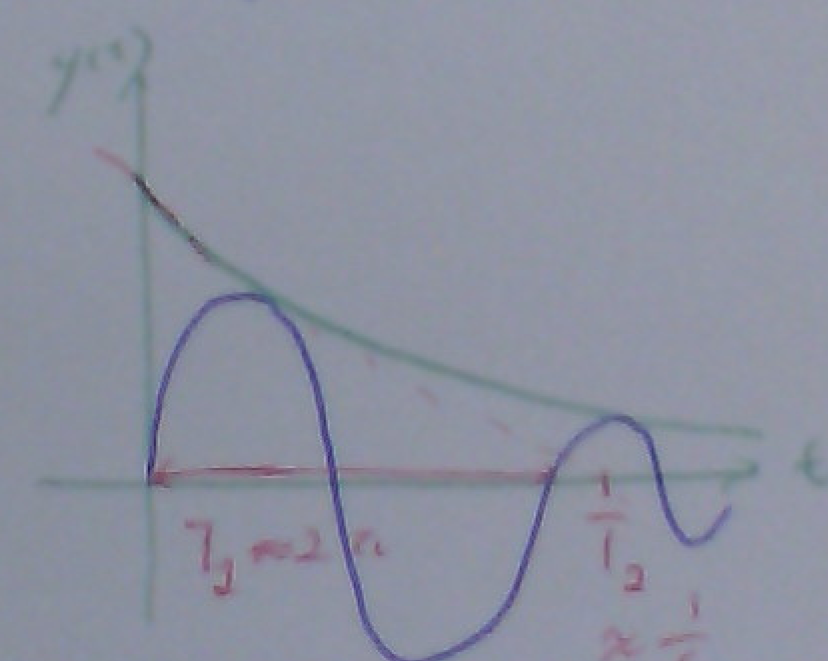

Relevant time scale: $T = \frac{1}{\varepsilon}$

$\boxed{\varepsilon << 1}$

(iii) $y'' + \varepsilon y' + y = 0 \quad \boxed{\varepsilon << 1} \Rightarrow y(t) = \frac{1}{\sqrt{1-\frac{\varepsilon^2}{4}}} e^{-\frac{\varepsilon t}{2}} \sin\left(t \underbrace{\sqrt{1-\frac{\varepsilon^2}{4}}}_{\approx 1}\right)$

$y(0) = 0$

$y'(0) = 1$




Perturbation Analysis problem (iii)

$$y(t) = \sum_{k=0}^{\infty} y_k(t)\,\varepsilon^k = y_0(t) + \varepsilon y_1(t) + \mathcal{O}(\varepsilon^2)$$

Substitute into ODE eqn (iii): (neglect $\mathcal{O}(\varepsilon^2)$ terms)

$$y_0'' + \varepsilon y_1'' + \varepsilon(y_0' + \cancelto{0}{\varepsilon y_1'}) + y_0 + \varepsilon y_1 = 0$$

$$y_0(0) + \varepsilon y_1(0) = 0$$

$$y_0'(0) + \varepsilon y_1'(0) = 1$$

Collect terms

$\varepsilon^0: y_0'' + y_0 = 0 \Rightarrow y(t) = \cancel{\sin(t)}$ $a\sin(t) + b\cos(t)$

$y_0(0) = 0$ $\Rightarrow b = 0 = y(0)$

$y_0'(0) = 1$ $a = 1 = y'(0)$

$\Rightarrow y_0(t) = \sin(t)$

$\varepsilon^1: y_1'' + y_0' + y_1 = 0$

$\Rightarrow y_1'' + y_1 = -y_0' = -\cos(t)$

$y_1(0) = 0$

$y_1'(0) = 0$

$\Rightarrow y_1(t) - \frac{1}{2} t \sin^2(t)$

$\Rightarrow y(t) = y_0(t) + \varepsilon y_1(t) = \sin(t) + \underbrace{\frac{1}{2}\varepsilon t \sin(t)}_{>0}$ hence it will go to infinity, instead of being damped! wrong behaviour.

$|y(t)| \to \infty \quad (t \to \infty)$

$\boxed{\text{Multiscale (two-scale)}}$

Explicitly let $y$ be a function of two time scale:

$$y(t) = \sum_{k=0}^{\infty} y_k(t_1(t), t_2(t))\varepsilon^k$$

$t_1(t) = t$

$t_2(t) = \varepsilon t$

$$y' = \frac{dy}{dt} = \frac{\partial y}{\partial t_1}\overbrace{\frac{\partial t_1}{\partial t}}^{=1} + \frac{\partial y}{\partial t_2}\overbrace{\frac{\partial t_2}{\partial t}}^{=\varepsilon}$$

$$= \frac{\partial y}{\partial t_1} + \frac{\partial y}{\partial t_2}\varepsilon$$

Substitute into ODE:

$\partial_t(\partial_{t_1} y + \partial_{t_2} y\,\varepsilon) + \varepsilon(\partial_{t_1} y + \varepsilon\partial_{t_2} y) + y = 0$ problem (ii)

$\partial_{t_1}^2 y + 2\varepsilon\partial_{t_1}\partial_{t_2} y + \varepsilon^2\partial_{t_2}^2 y + \varepsilon\partial_{t_1} y + \varepsilon^2\partial_{t_2} y + y = 0$

$\partial_{t_1}^2(y_0 + \varepsilon y_1) + 2\varepsilon\partial_{t_1}\partial_{t_2}(y_0 + \varepsilon y_1) + \varepsilon\partial_{t_1}(y_0 + \varepsilon y_1) + y_0 + \varepsilon y_1 \approx 0$

$y_0 + \varepsilon y_1 \big|_{t=0} = 0$

$\underbrace{\underbrace{\partial_{t_1}(y_0 + \varepsilon y_1)}_{\approx y} + \varepsilon \underbrace{\partial_{t_2}(y_0 + \varepsilon y_1)}_{\approx y}}_{d_t y} \Big|_{t=0} = 1$

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$\varepsilon^0$: $\partial_{t_1}^2 y_0 + y_0 = 0 \Rightarrow y_0(t) = a_0(t_2)\sin(t_1) + b_0(t_2)\cos(t_1)$

$t_2 = \varepsilon t$

$y_0(0) = 0$

$\partial_{t_1} y_0(0) = 1$

$y_0(0) = b_0(0) = 0 \quad (1)$

$\partial_{t_1} y_0(0) = a_0(0) = 1 \quad (2)$

$\varepsilon^1$:

~~$\partial_{t_1}^2 y_1 + 2\partial_{t_2} y_2$~~

$\partial_{t_1}^2 y_1 + 2\partial_{t_1}\partial_{t_2} y_0 + \partial_{t_1} y_0 + y_1 = 0$

$\Rightarrow \partial_{t_1}^2 y_1 + y_1 = -2\partial_{t_1}\partial_{t_2} y_0 - \partial_{t_1} y_0$

$[\partial_{t_1} y_0 = a_0(t_2)\cos(t_1) - b_0(t_2)\sin(t_1)]$

$= -2(a_0'(t_2)\cos(t_1) + b_0'(t_2)\sin(t_1)) \underbrace{- a_0(t_2)\cos(t_1) + b_0(t_2)\sin(t_1)}_{\partial_{t_1} y_0(t)}$

$\Rightarrow \partial_{t_1}^2 y_1 + y_1 = -\underbrace{(2a_0' + a_0)}_{\stackrel{!}{=}0}\cos(t_1) + \underbrace{(2b_0' + b_0)}_{\stackrel{!}{=}0}\sin(t_1)$

modelling assumptions based on physical observation of system.

kill growth terms

$2a_0' + a_0 = 0 \Rightarrow a_0(t_2) = C e^{-\frac{t_2}{2}}$

$(2) \Rightarrow a_0(0) = 1 \Rightarrow C = 1$

$\left.\begin{array}{l} 2b_0' + b_0 = 0 \\ b_0(0) = 0 \end{array}\right\} b_0 \equiv 0$

$\Rightarrow y_0(t) = e^{-\frac{t_2}{2}} \sin(t)$, $t_2 = \varepsilon t$

$= e^{-\frac{\varepsilon t}{2}} \sin(t)$

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Previously:

Linearized (averaged) LGA

$$\left.\frac{\partial C_i(N)}{\partial N_j}\right|_{u=0}$$ → collision operator of averaged LGA

$$N_i(\underline{r}+\underline{c}_i, t+1) = N_i(\underline{r},t) + C_{ij}^{(0)}(N_j(\underline{r},t) - N_j^{(eq)})$$

in LBM $C_i(N)$ and $N_j^{(eq)}$ is chosen for consistency with conservation laws. Here, strictly no relation with LGA anymore.

Conservation:

$$C_i^{(lin)}(N^{(eq)}) = 0$$

$$\sum_i C_i^{(lin)} = 0$$

$$\sum_i c_i C_i^{(lin)} = 0$$

$$f_i(\underline{r}+\underline{c}_i, t+1) = f_i(\underline{r},t) + \omega\underbrace{\left(f_i^{(eq)}(\underline{r},t) - f_i(\underline{r},t)\right)}_{C_i}$$

$$f_i^{(eq)} = \rho w_i\left(1 + \frac{\underline{c}_i\cdot\underline{u}}{c_s^2} - \frac{u^2}{2c_s^2} + \frac{1}{2}\cdot\frac{(\underline{c}_i\cdot\underline{u})^2}{(RT)^2}\right) \; ; \; c_s^2 = RT$$

quadrature weights, eventually.

Note:

$$\rho(\underline{r},t) = \sum_i f_i(r,t)$$

$$\rho\underline{u} = \sum_i \underline{c}_i f_i$$

Determine $w_i$ s.th.

$$\sum_i f_i^{(eq)} c_{i,1}^m c_{i,2}^n = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^m c_2^n \, dc_1 dc_2 \quad ; \quad \underline{c}_i = (c_{i,1} \;\; c_{i,2})^T$$

up to some degree m, n.

$$\tilde{f}^{(eq)} = \frac{\rho}{2\pi RT} e^{-\frac{c^2}{RT}}\left\{1 + \frac{\underline{c}\cdot\underline{u}}{RT} - \frac{u^2}{RT} + \frac{1}{2}\frac{(\underline{c}\cdot\underline{u})^2}{(RT)^2}\right\} \; ;$$

known:

$$\int_{\mathbb{R}^2} \tilde{f}^{(eq)} \, d\underline{c} = \rho$$

$$\int_{\mathbb{R}^2} \tilde{f}^{(eq)} \underline{c} \, d\underline{c} = \rho\underline{u}$$

In particular, then we have

$$\sum_i f_i^{(eq)} = \rho = \sum_i f_i \Rightarrow \sum_i C_i = 0$$

$$\sum_i \underline{c}_i f_i^{(eq)} = \rho\underline{u} = \sum_i f_i \underline{c}_i \Rightarrow \sum_i \underline{c}_i C_i = 0$$

Recall: Gauss-Hermite Quadrature:

$$\int_{\mathbb{R}} e^{-x^2} g(x) = \sum_{i=1}^{n} w_i g(x_i) + R_n$$

Set $\underline{c} = \sqrt{2RT}\,\underline{\xi}$

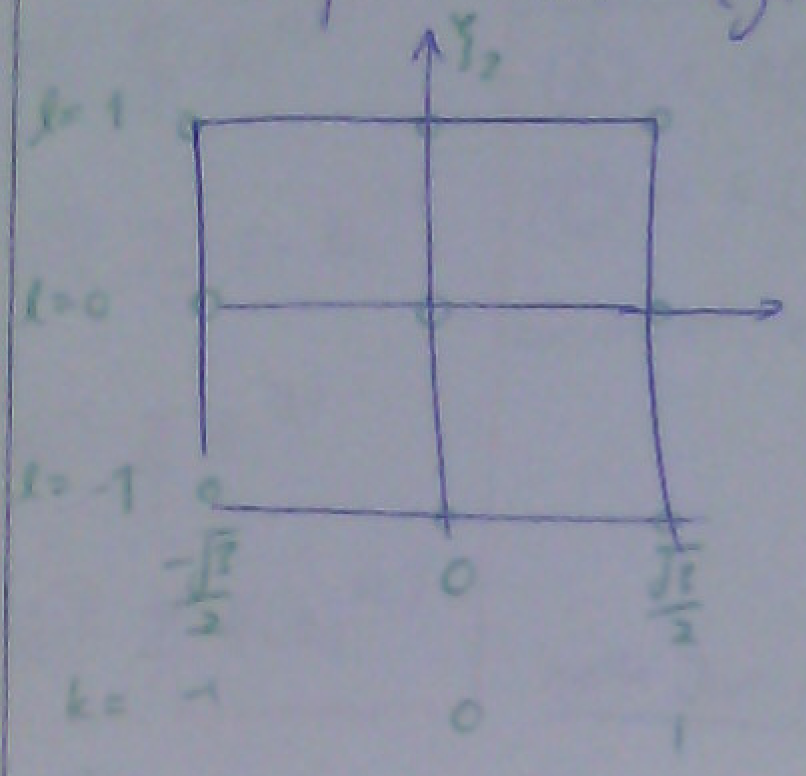
Then $$I = \int_{\mathbb{R}^2} \tilde{f}^{(eq)} c_1^m c_2^n \, dc_1 dc_2$$

$$= \frac{\rho}{\pi}(2RT)^{\frac{m+n}{2}} \int_{\mathbb{R}^2} \xi_1^m \xi_2^n e^{-\xi^2}\left(1 + \frac{\sqrt{2}\,\underline{\xi}\cdot\underline{u}}{\sqrt{RT}} - \frac{u^2}{2RT} + \frac{(\underline{\xi}\cdot\underline{u})^2}{RT}\right) d\xi_1 d\xi_2$$

LBM Lecture 23rd Dec 2016 (1)

Use 3 point Rule: (Gauss – Hermite)

LBM $f_i^{(eq)} = \rho w_i \left(1 + \frac{c_i \cdot u}{c_s^2} - \frac{u^2}{2c_s^2} + \frac{1}{2} \cdot \frac{(c_i \cdot u)^2}{(RT)^2}\right)$




$w_0 = \frac{2\sqrt{\pi}}{3}$

$w_{-1} = w_1 = \frac{\sqrt{\pi}}{6}$

$$\Rightarrow I \approx \rho (2RT)^{\frac{m+n}{2}} \sum_{k,l=-1}^{1} \frac{w_k w_l}{\pi} \xi_{1,k}^m \xi_{2,k}^n \left\{ 1 + \frac{\sqrt{2}(\xi_{1,k} u_1 + \xi_{2,l} u_2)}{\sqrt{RT}} - \frac{u^2}{2RT} + \frac{(\xi_{1,k} u_1 + \xi_{2,l} u_2)^2}{RT} \right\}$$

<u>Note</u>: $\xi_{1,k} u_1 + \xi_{2,k} u_2$

$= \sqrt{\frac{3}{2}} (k u_1 + l u_2)$

$= \frac{\sqrt{3}}{\sqrt{2}} (\tilde{c}_{k,l} \cdot \underline{u})$ ; $\tilde{c}_{k,l} = (k,l)^T$

<u>and</u>: $\frac{w_k w_l}{\pi} = \begin{cases} 4/9 & k = l = 0 \\ 1/9 & k=0 \;\; l \neq 0 \\ & l=0 \;\; k \neq 0 \\ 1/36 & |k| = |l| = 1 \end{cases}$

Set $\tilde{u} = \frac{u}{\sqrt{2RT}}$

$$f_i^{(eq)} = \begin{cases} 4/9\, \rho \{1 - \frac{3}{2} u^2\} & , i = 0 \\ 1/9\, \rho \{1 + 3 \tilde{c}_i \cdot \tilde{\underline{u}} + \frac{9}{2}(\tilde{c}_i \cdot \tilde{\underline{u}})^2 - \frac{3}{2} \tilde{u}^2\} & , i = 1,2,3,4 \\ 1/36\, \rho \{ \dots \} & , i = 5,6,7,8. \end{cases}$$

moments:

$\rho = \sum f_i$

$\rho u = \sum c_i f_i$ Claim! these quantities satisfies NS-equations.

<u>Multiscale expansion</u>

<u>Recall</u>: LBM D2Q9, 2D, 9 point Quadrature

(1) $f_i(\underline{x} + c_i, t+1) = f_i(\underline{x}, t) + \omega (f_i(\underline{x}, t) - f_i^{(eq)}(\underline{x}, t))$

(2) $\sum_{i=0}^{8} f_i^{(eq)} = \sum_{i=0}^{8} f_i = \rho$

(3) $\sum_{i=0}^{8} c_i f_i^{(eq)} = \sum_{i=0}^{8} c_i f_i = \rho \underline{u}$

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**Relevant Scales:** (spatial and temporal)

Let $\varepsilon = \frac{1}{N}$ # nodes per dim.

① Lattice "knudsen" number $= \frac{\Delta x}{L} = O(\varepsilon) = O\left(\frac{1}{N}\right)$

② (i) convective scale $O(N)$

(ii) diffusive scale $O(N^2)$

**Scaled coordinates:**

(a) – indicates power of $\varepsilon$

$r_\alpha = \varepsilon x_\alpha$

$t^{(1)} = \varepsilon t \qquad t = N = \frac{1}{\varepsilon} \Rightarrow t^{(1)} = 1$

$t^{(2)} = \varepsilon^2 t \qquad t = N^2 = \frac{1}{\varepsilon^2} \Rightarrow t^{(2)} = 1$

$$\left.\begin{aligned} \frac{\partial}{\partial t} &= \frac{\partial}{\partial t^{(1)}}\frac{\partial t^{(1)}}{\partial t} + \frac{\partial}{\partial t^{(2)}}\frac{\partial t^{(2)}}{\partial t} \\ &= \varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)} \\ \frac{\partial}{\partial r_\alpha} &= \varepsilon \partial_\alpha^{(1)} \end{aligned}\right\} (**)$$

**Need to expand:**

$$f_i = \sum_{k=0}^{\infty} \varepsilon^k f_i^{(k)} = \sum_{k=0}^{\infty} \varepsilon^k f^{(k)}\left(r^{(1)}(r), t^{(1)}(t), t^{(2)}(t)\right)$$

$$\left. f_i = f_i^{(0)} + \varepsilon f_i^{(1)} \Big| + \varepsilon^2 f_i^{(2)} + \dots \right\} (***)$$

neglected.

Taylor expansion:

$$f_i(\underline{r} + \underbrace{\underline{c}_i \Delta t}_{\Delta r_\alpha}, t + \Delta t) = f_i(\underline{r}, t) + \partial r_\alpha f_i c_{i\alpha} \Delta t + \partial_t f_i \Delta t + \frac{1}{2}(\Delta t)^2 \big(\partial_t \partial_t f_i + 2 c_{i\alpha} \partial r_\alpha \partial_t f_i + c_{i\alpha} c_{i\beta} \partial_\alpha \partial r_\beta f_i\big) \quad (*)$$

summation

free index

substitute $(*)$ into (1)

$$\Rightarrow \partial r_\alpha f_i c_{i,\alpha} \Delta t + \partial_t f_i \Delta t + \frac{(\Delta t)^2}{2}\{\dots\} - \omega(f_i^{(eq)} - f_i) = 0$$

substitute (**) (***) into ↑

$$\Rightarrow E_i^{(0)} + \varepsilon E_i^{(1)} + \varepsilon^2 E_i^{(2)} \Big| + \dots = 0$$

$E_i^{(m)}$ contain only such terms $\partial_t^{(k)} f_i^{(l)}$ with $k + l = m$ ($\varepsilon$ that has power up to m)

$E_i^{(0)} \equiv 0$ if $f_i^{(0)} = f_i^{(eq)}$

$E_i^{(1)} = \partial_\alpha^{(1)} f_i^{(0)} c_{i\alpha} \Delta t + \partial_t^{(1)} f_i^{(0)} \Delta t + \omega f_i^{(1)}$

$E_i^{(2)} = \partial_\alpha^{(1)} f_i^{(1)} c_{i\alpha} \Delta t + \Delta t \, \partial_t^{(2)} f^{(0)} + \Delta t \, \partial_t^{(1)} f^{(1)} + \frac{1}{2}(\Delta t)^2 \left(\partial_t^{(1)} \partial_t^{(1)} f_i^{(0)} + 2 c_{i\alpha} \partial_\alpha^{(1)} \partial_t^{(1)} f_i^{(0)} + c_{i\alpha} c_{i\beta} \partial_\alpha^{(1)} \partial_\beta^{(1)} f_i^{(0)}\right) + \omega f^{(2)}$

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Moments:

A $\sum_i E_i^{(1)}$

B $\sum_i \underline{c}_i E_i^{(1)}$

C $\sum_i E_i^{(2)}$

D $\sum_i \underline{c}_i E_i^{(2)}$

claim: ← could be erroneous!

A $+ \varepsilon$ B $= 0$

C $+ \varepsilon$ D $= 0$

consistent with Navier-stokes.

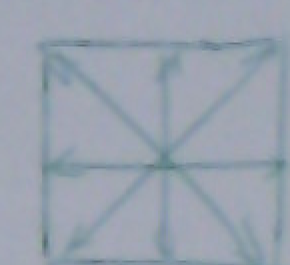
30th Jan 2017

Review

Multiscale Expansion.

(LBM)

(1) $f_i(\underline{r}+\underline{c}_i\Delta t, t+\Delta t) = f_i(\underline{r},t) + \omega(f_i^{eq}(\underline{r},t) - f_i(\underline{r},t))$ , $i=0,\dots,9$



$$f_i^{(eq)} = \rho w_i \left(1 + 3(\underline{c}_i\cdot\underline{u}) - \frac{3}{2}u^2 + \frac{9}{2}(\underline{c}_i\cdot\underline{u})^2\right)$$

(2) $\sum_{i=0}^{8} f_i(\underline{r},t) = \sum_{i=0}^{8} f_i^{(eq)}(\underline{r},t) = \rho$

(3) $\sum_{i=0}^{8} \underline{c}_i f_i(\underline{r},t) = \sum_{i=0}^{8} \underline{c}_i f_i^{(eq)}(\underline{r},t) = \rho\underline{u}$

Relevant (spatial & temporal) scales

Let $\varepsilon = \frac{1}{N}$

(*) "Lattice Knudsen" number $\frac{\Delta x}{L} = O(N^{-1}) = O(\varepsilon)$ ← char length scale

(*) (i) Convective timescale $O(N)$

(ii) diffusive timescale $O(N^2)$

Introduce Scaled Coordinates

$\underline{r}^{(1)} = \varepsilon \underline{r}$ $\quad r = N \Rightarrow r^{(1)} = 1$

$t^{(1)} = \varepsilon t$ $\quad t = N \Rightarrow t^{(1)} = 1$

$t^{(2)} = \varepsilon^2 t$ $\quad t = N^2 \Rightarrow t^{(2)} = 1$

we will set $f_i = \sum_{k=0}^{\infty} \varepsilon^k f_i^{(k)}$

$$f_i^{(k)} = f_i^{(k)}(r^{(1)}, t^{(1)}(t), t^{(2)}(t))$$

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$$\frac{\partial}{\partial t} = \frac{\partial t^{(1)}}{\partial t}\frac{\partial}{\partial t^{(1)}} + \frac{\partial t^{(2)}}{\partial t}\frac{\partial}{\partial t^{(2)}}$$

$$\Rightarrow \partial_t = \varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)}$$

$$\frac{\partial}{\partial r} = \varepsilon \frac{\partial}{\partial r^{(1)}} \qquad (4)$$

$$\Rightarrow \partial_{r_\alpha} = \varepsilon \partial^{(1)}_{r_\alpha} \quad ; \alpha = 1, 2.$$

hence: $f_i = f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \dots \qquad (5)$

Note: $\sum_i f_i^{(k)(1)} = 0 \qquad k \geq 1 \quad \left(f^{(0)} = f^{(eq)}\right)$

$\sum_i c_i f_i^{(k)(1)} = 0$

---

$$f_i(r + c_i t, t + \Delta t) = f_i(r,t) + c_{i,\alpha}\Delta t\, \partial_\alpha f_i + \partial_t f_i \Delta t + \frac{\Delta t^2}{2}\left\{\partial_t \partial_t f_i + 2 c_{i,\alpha} \partial_\alpha \partial_t f_i + c_{i,\alpha} c_{i,\beta} \partial_\alpha \partial_\beta f_i\right\} + O(\Delta t^3) \qquad (6)$$

summation.

i is still free index.

Substitute (6) into (1)

$$c_{i,\alpha}\Delta t\, \partial_\alpha f_i + \Delta t\, \partial_t f_i + \frac{\Delta t^2}{2}\{\dots\} - \omega(f^{(eq)} - f_i) \approx 0 \qquad (7)$$

Substitute (4), (5) into (7)

$$(7) \Rightarrow E_i^{(0)} + \varepsilon E_i^{(1)} + \varepsilon^2 E_i^{(2)} + \dots$$

where each $E^{(k)}$ contains terms like

$$\partial_t^{(l)} f^{(m)} \quad \text{s.th. } l + m = k$$

Solve $f^{(0)}, f^{(1)}, f^{(2)}$, etc. by ... by equating $E_i^{(k)} = 0$.

$$E_i^{(0)} = f^{(0)} - f^{(eq)}$$

$$E_i^{(1)} = c_{i,\alpha}\Delta t\, \partial_\alpha^{(1)} f_i^{(0)} + \Delta t\, \partial_t^{(1)} f_i^{(0)} + \omega f^{(1)}$$

$$E_i^{(2)} = \Delta t\, \partial_t^{(1)} f_i^{(1)} + \Delta t\, \partial_t^{(2)} f_i^{(0)} + c_{i,\alpha}\Delta t\, \partial_\alpha^{(1)} f^{(1)} + \frac{(\Delta t)^2}{2}\left\{\partial_t^{(1)}\partial_t^{(1)} f_i^{(0)} + 2 c_{i,\alpha}\partial_\alpha^{(1)}\partial_t^{(1)} f_i^{(0)} + c_{i,\alpha}c_{i,\beta}\partial_\alpha^{(1)}\partial_\beta^{(1)} f_i^{(0)}\right\} - \omega f^{(2)}$$

Moments:

(A) $\sum_{i=0}^{8} E_i^{(1)}$ (C) $\sum E_i^{(2)}$

(B) $\sum c_i E_i^{(1)}$ (D) $\sum c_i E_i^{(2)}$

LBM

27th Jan 2017

2

Claim:

$$\sum E_i^{(1)} + \varepsilon E_i^{(2)} = 0 \qquad \text{"gives" N-S.}$$

$$\sum c_i \left(E_i^{(1)} + \varepsilon E_i^{(2)}\right) = 0$$

by conservation. note that $f^{(0)} = f^{(eq)}$

A $\frac{1}{\Delta t} \sum_i E_i^{(1)} = \sum_i \partial_t^{(1)} f_i^{(0)} + c_{i,\alpha} \partial_\alpha^{(1)} f_i^{(0)} + \cancel{\frac{\omega}{\Delta t} f_i^{(1)}}^{\,0}$

$$= \partial_t^{(1)} \underbrace{\left(\sum_i f_i^{(0)}\right)}_{\rho} + \partial_\alpha^{(1)} \underbrace{\left(\sum_i c_{i,\alpha} f_i^{(0)}\right)}_{\rho u_\alpha}$$

$$= \partial_t^{(1)} \rho + \partial_\alpha^{(1)} (\rho u_\alpha)$$

0 by conservation.

B $\frac{1}{\Delta t} \sum c_i E_i^{(1)} = \sum_i c_{i,\alpha} \partial_t^{(1)} f_i^{(0)} + \sum_i c_{i,\alpha} c_{i,\beta} \partial_\beta^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t} \cancel{\sum_i f_i^{(1)} c_{i,\alpha}}^{\,0}$

$$= \partial_t^{(1)} \underbrace{\left(\sum_i c_{i,\alpha} f_i^{(0)}\right)}_{\rho u_\alpha} + \partial_\beta^{(1)} \underbrace{\left(\sum_i c_{i,\alpha} c_{i,\beta} f_i^{(0)}\right)}_{P_{\alpha\beta}^{(0)}}$$

C $\frac{1}{\Delta t} \sum_i E_i^{(2)} = \partial_t^{(2)} \rho + \frac{\Delta t}{2} \left\{ \partial_t^{(1)} \partial_t^{(1)} \rho + 2 \partial_\alpha^{(1)} \partial_t^{(1)} \rho u_\alpha + \partial_\alpha^{(1)} \partial_\beta^{(1)} P_{\alpha\beta}^{(0)} \right\} - \frac{\omega}{\Delta t} f^{(2)}$

$$= \partial_t^{(2)} \rho + \frac{\Delta t}{2} \Big[ \partial_t^{(1)} \underbrace{\left(\partial_t^{(1)} \rho + \partial_\alpha^{(1)} \rho u_\alpha\right)}_{\mathcal{O}(\varepsilon) \approx 0} + \partial_t^{(1)} \partial_\alpha^{(1)} \rho u_\alpha + \partial_\alpha^{(1)} \partial_\beta^{(1)} P_{\alpha\beta}^{(1)} \Big]$$

→ neglect because

$$= \partial_t^{(2)} \rho + \frac{\Delta t}{2} \partial_\alpha^{(1)} \underbrace{\left\{ \partial_t^{(1)} \rho u_\alpha + \partial_\beta^{(1)} P_{\alpha\beta} \right\}}_{\mathcal{O}(\varepsilon) \approx 0}$$

$0 = \varepsilon \sum E_i^{(1)} + \varepsilon^2 \sum E_i^{(2)}$, this will give $\varepsilon = 3$. term dropped.

$$\to \frac{\varepsilon}{\Delta t} \sum E_i^{(1)} + \frac{\varepsilon^2}{\Delta t} \sum E_i^{(2)} = \varepsilon \partial_t^{(1)} \rho + \varepsilon^2 \partial_t^{(2)} \rho + \varepsilon \partial_\alpha^{(1)} (\rho u_\alpha)$$

C A

$$= \partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0$$

Need to finish moment B

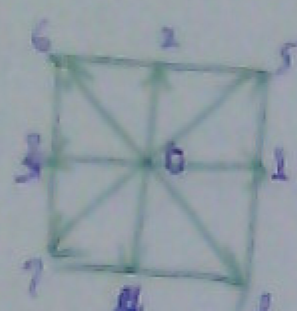
$$\text{B} = \frac{1}{\Delta t} \sum c_{i,\alpha} E_i^{(1)} = \partial_t^{(1)} \rho u_\alpha + \partial_\beta^{(1)} \underbrace{\left(c_{i,\alpha} c_{i,\beta} f_i^{(0)}\right)}_{P_{\alpha\beta}^{(0)}}$$

$$P_{\alpha\beta}^{(0)} = \sum c_{i,\alpha} c_{i,\beta} \rho w_i \left\{ 1 + 3 (c_i \cdot u) - \frac{3}{2} u^2 + \frac{9}{2} (c_i \cdot u)^2 \right\}$$

$$= P_{\alpha\beta}^{(0,1)} + P_{\alpha\beta}^{(0,2)} + P_{\alpha\beta}^{(0,3)} + P_{\alpha\beta}^{(0,4)}$$

LBM ... 23rd Dec 2016

$$\frac{\partial}{\partial t} \quad P_{\alpha\beta}^{(0,1)} = \cancel{\beta}\,\rho \sum_i w_i \, c_{i,\alpha} \, c_{i,\beta} = \rho \frac{1}{3} \delta_{\alpha\beta}$$



$\Rightarrow \partial_t$ $\quad w_0 = \frac{4}{9}$ $\quad w_i^{\circ} = \frac{1}{9} \quad i = 1, \dots, 4$

$\frac{\partial}{\partial r}$ $\quad w_i^{\circ} = \frac{1}{36} \quad i = 5, \dots, 8$

$\Rightarrow \partial_{r_1}$ $\quad$ e.g. $\alpha = \beta = 1$

hence
$$\sum w_i \, c_{i,\alpha=1}^{2} \to \{0,1\} = 2 \cdot \frac{1}{9} + \frac{4}{36} = \frac{1}{3}$$

No Recall: $c_{i,\alpha}^* = c_0^*$ $\qquad (c_s^*)^2 = RT^*$

dimensional

$$\left(\frac{c_0^*}{c_s^*}\right)^2 = 3 \quad \text{(ref. chap 10)}$$

$$\Rightarrow \frac{1}{3} = \left(\frac{c_s^*}{c_0^*}\right)^2 = \frac{RT^*}{c_0^{*2}} \quad , \text{Also} = \rho = \frac{\rho^*}{\rho_{ref}}$$

$$\Rightarrow P_{\alpha\beta}^{(0,1)} = \frac{\rho^*}{\rho_{ref}} \cdot \frac{RT^*}{(c_0^*)^2} \delta_{\alpha\beta} = \frac{p^*}{p_{ref}} \frac{\delta_{\alpha\beta}}{(c_0^*)^2} = p \, \delta_{\alpha\beta}$$

Also:

$$P_{\alpha\beta}^{(0,2)} = 3 \rho u_\gamma \overbrace{\sum w_i c_{i,\alpha} c_{i,\beta} c_{i,\gamma}}^{\text{vanishes}} = 0$$

$$P_{\alpha\beta}^{(0,3)} = -\frac{3}{2}(u_1^2 + u_2^2) \rho \overbrace{\sum w_i \, c_{i,\alpha} \, c_{i,\beta}}^{\frac{1}{3}\delta_{\alpha\beta}} = -\frac{1}{2}(u_1^2 + u_2^2) \rho \, \delta_{\alpha\beta}$$

$$P_{\alpha\beta}^{(0,4)} = \frac{3}{2} \rho \sum_i w_i \, c_{i,\alpha} \, c_{i,\beta} \, \underbrace{(c_i \cdot u)^2}_{u_1^2 c_{i,1}^2 + 2 c_{i,1} c_{i,2} u_1 u_2 + c_{i,2}^2 u_2^2} \Rightarrow P_{\alpha\beta}^{(0,4)} = \begin{cases} \frac{3}{2}\rho u_1^2 + \frac{1}{2}\rho u_2^2 & \alpha = \beta = 1 \\ \rho u_\alpha u_\beta & \alpha \neq \beta \\ \frac{1}{2}\rho u_1^2 + \frac{3}{2}\rho u_2^2 & \alpha = \beta = 2 \end{cases}$$

$$P_{11}^{(0)} = p + \frac{1}{2}(u_1^2 + u_2^2)\rho + \frac{3}{2}\rho u_1^2 + \frac{1}{2}\rho u_2^2$$
$$= p + \rho u_1^2$$

Similarly, $\quad P_{\alpha\beta}^{(0)} = \rho u_\alpha u_\beta \quad (\alpha \neq \beta)$

$$P_{22}^{(0)} = p + \rho u_2^2$$

$$P_{\alpha\beta}^{(0)} = p \, \delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

$$\frac{1}{\delta t} \sum c_{i,\alpha} E_i^{(1)} = \partial_t^{(1)}(\rho u_\alpha) + \partial_\beta^{(1)} P_{\alpha\beta}^{(0)} = \partial_t^{(1)}(\rho u_\alpha) + \partial_\alpha^{(1)} p + \partial_\beta^{(1)}(\rho u_\alpha u_\beta)$$

LBM tutorial

26th Jan 2017

German Research School for Simulation Sciences

$A \left\{ \sum_i E^{(1)} \right. \quad \Rightarrow \varepsilon A + \varepsilon^2 B = 0 \quad = \partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\beta)$

$B \sum_i c_{i\alpha} E_i^{(1)} \qquad \varepsilon C + \varepsilon^2 D = 0$ today!

$C \sum_i E_i^{(2)} \qquad \partial_t^{(1)}(\rho u_\alpha) + \partial_\beta^{(1)}(\rho u_\alpha u_\beta) + \partial_\alpha P$

$D \sum_i c_{i\alpha} E_i^{(2)}$

as conservation states $\sum f_i^{(k)} = 0 \Leftarrow \sum f^{(0)} = \rho$, $k>0$

$\Downarrow$

$\sum c_{i\alpha} f_i^{(k)} = 0$

$$\frac{1}{\Delta t} E_i^{(2)} = \partial_t^{(1)} f_i^{(1)} + \partial_t^{(2)} f_i^{(0)} + c_{i\alpha}\partial_\alpha f_i^{(1)} + \frac{1}{2}\Delta t\left(\partial_t^{(1)}\partial_t^{(1)} f_i^{(0)} + 2c_{i\alpha}\partial_t^{(1)}\partial_\alpha^{(1)} f_i^{(0)} + c_{i\beta}c_{i\alpha}\partial_\alpha^{(1)}\partial_\beta^{(1)} f_i^{(0)}\right) + \frac{\omega}{\Delta t} f_i^{(2)}$$

$$\Rightarrow \frac{1}{\Delta t}\sum_i c_{i\alpha} E_i^{(2)} = \partial_t^{(1)}(\rho u_\alpha) + \partial_\beta^{(1)}\sum_i c_{i\alpha}c_{i\beta} f_i^{(1)} + \frac{1}{2}\Delta t\Big(\partial_t^{(1)}\partial_t^{(1)}(\rho u_\alpha) + 2\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \underbrace{\partial_\beta^{(1)}\partial_\gamma^{(1)}\sum_i c_{i\alpha}c_{i\beta}c_{i\gamma} f_i^{(0)}}_{(**)}\Big)$$

$P_{\alpha\beta} = \sum_i c_{i\alpha} c_{i\beta} f_i^{(0)}$

$$\frac{1}{\Delta t} E^{(1)} = \partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)} + \frac{\omega}{\Delta t} f_i^{(1)} \quad (*)$$

formally let $\varepsilon \to 0$ in $\varepsilon A + \varepsilon^2 B = 0$

$$f_i^{(1)} = -\frac{\Delta t}{\omega}\left\{\partial_t^{(1)} f_i^{(0)} + c_{i\alpha}\partial_\alpha^{(1)} f_i^{(0)}\right\}$$

$$\Rightarrow \frac{1}{\Delta t}\sum_i c_{i\alpha} E_i^{(2)} = \partial_t^{(2)}(\rho u_\alpha) - \frac{\Delta t}{\omega}\partial_\beta^{(1)}\partial_t^{(1)}\underbrace{\sum_i c_{i\alpha}c_{i\beta} f_i^{(0)}}_{P_{\alpha\beta}} - \frac{\Delta t}{\omega}\partial_\beta^{(1)}\partial_\gamma^{(1)}\sum_i c_{i\alpha}c_{i\beta}c_{i\gamma} f_i^{(0)} + \frac{1}{2}\Delta t\left\{ \overset{**}{\cdots} \right\}$$

$$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(1 - \frac{1}{\omega}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \Delta t\left(\frac{1}{2} - \frac{1}{\omega}\right)\partial_\beta^{(1)}\partial_\gamma^{(1)}\sum_i c_{i\alpha}c_{i\beta}c_{i\gamma} f_i^{(0)}$$

$$+ \underbrace{\frac{1}{2}\Delta t\,\partial_t^{(1)}\partial_t^{(1)}(\rho u_\alpha)}_{\text{disappears } (\varepsilon \to 0?)}$$

Recall: momentum:

$$\partial_t(\rho u_\alpha) + \underbrace{\partial_\beta(\rho u_\alpha u_\beta) + \partial_\alpha P}_{\partial_\beta P_{\alpha\beta}} = O(\varepsilon)$$

$$H^{(q)} = \sum_{x,t} \boxed{\sum_i h_i(f_i(x,t))} \to H$$
$$\underbrace{\sum_i h_i(f_i(x,t))}_{\tilde{h}_i(x,t)}$$

s.th. $\frac{dH}{dt} \le 0$

Basics (Cont'd):

**LGA**

→ Model ⇝ { streaming; collision – constraints: mass conservation etc.

→ Equilibrium: stochastic, statistical equilibrium possible. Fermi-dirac equ.
↳ H-Theorem

→ Short comings.

→ (Intermediate Models)

$$f^{(q)} = \arg\min \left\{ H^{(q)}(t) : \rho = \sum f_i^{(0)} ; \ \sum c_i f_i^{(0)} \right\} = \rho \underline{u}$$

introduce Lagrangian:

$$H_L := \sum_i h_i(f_i) - a\left(\sum f_i - \rho\right) + \underline{b}\cdot\left(\sum c_i f_i - \rho \underline{u}\right)$$

optimality condition:

$$\frac{\partial H_L}{\partial f_i} = h_i'(f_i) - a - c_i \underline{b} \overset{!}{=} 0$$

$$\Rightarrow f_i^{(0)} = (h_i')^{-1}(a + \underline{b}\cdot \underline{c}_i) \qquad \sum_i f_i^{(0)} = \rho \qquad \sum_i \underline{c}_i f_i^{(0)} = \rho \underline{u}$$

**LBM** (Derivation) ← should know how.

→ LB equation. → should write down.

→ moments $\left(\sum f_i = \rho,\ \sum \underline{c}_i f_i = \rho \underline{u}\right)$

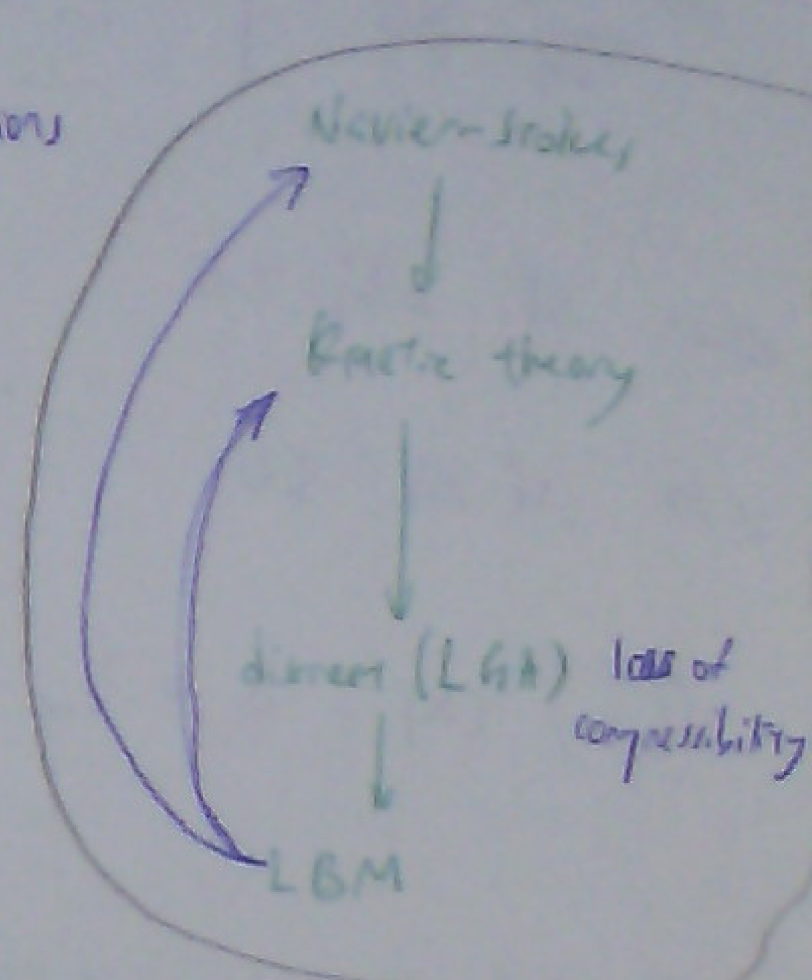
→ Multiscale expansion → should know concept perturbation, Taylor expansion around the equilibrium. ⇓ NS small compressibility

→ Viscosity ← fine parameter

– Stability ← linearized stability analysis approx. (incomp. NS)

– Boundary conditions

– H-Theorem.




Show: H is non-increasing during collision:

$$f_i(t) + \omega(f_i^{(0)}(t) - f_i(t)) = f(t+1)$$

Recall: fundamental theorem of calculus:

$$\int_0^1 \frac{\partial}{\partial s} g(t+s)\, ds \underset{t+s=\xi}{=} \int_t^{t+1} g'(\xi)\, d\xi = g(t+1) - g(t)$$

$$\boxed{\text{Define: } f_i(t+s) = f_i(t) + s\omega(f_i^{(0)}(t) - f_i(t))} \qquad 0 \le s \le 1 \qquad \sum f_i(t+s) = \rho(t+s),\ \rho\underline{u} \text{ similar}$$

Let $0 < \omega < 1$ generally $0 < \omega < 2$

Then

$$\tilde{h}_i(t+1) - \tilde{h}_i(t) = h_i(f_i(t+1)) - h_i(f_i(t)) = \int_0^1 \frac{\partial}{\partial s}\{h_i(f_i(t+s))\}\, ds$$

$$= \int_0^1 \frac{\partial}{\partial s}\{h_i(f_i(t+s))\} + a\frac{\partial}{\partial s}\underbrace{\left(\sum f_i - \rho\right)}_{=0}\Big|_{t+s} + \underline{b}\frac{\partial}{\partial s}\left(\sum \underline{c}_i f_i - \rho\underline{u}\right)\Big|_{t+s} ds$$

$$= \int_0^1 \left(\frac{\partial h_i}{\partial f_i} - a\frac{\partial}{\partial f_i}\left(\sum f_i - \rho\right) - \underline{b}\cdot\frac{\partial}{\partial f_i}\left(\sum c_i f_i - \rho\underline{u}\right)\right)\frac{d}{ds} f_i(t+s)\, ds$$

$$= \int_0^1 (h_i' - a - \underline{b}\cdot\underline{c}_i)\,\omega\,(f_i^{(0)} - f_i)\Big|_{t+s}\, ds$$

$$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(\frac{1}{2}-\frac{1}{\omega}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \Delta t\left(\frac{1}{2}-\frac{1}{\omega}\right)\partial_\beta^{(1)}\partial_\gamma^{(1)} \sum c_{i,\alpha} c_{i,\beta} c_{i,\gamma} f_i^{(0)}$$

$$P_{\alpha\beta} = \partial_\alpha p = \partial_\beta \rho c_s^2 + \underbrace{O(h^2)}_{\to 0} \qquad f_i^{(0)} \approx \rho w_i \left(1 + \frac{c_{i,\alpha} u_\alpha}{c_s^2}\right) + \underbrace{O(h^2)}_{\to 0}$$

$$\Rightarrow \partial_\beta^{(1)}\partial_\gamma^{(1)} \sum c_{i,\alpha} c_{i,\beta} c_{i,\gamma} \rho w_i \left(1 + \frac{c_{i,\sigma} u_\sigma}{c_s^2}\right)$$

odd moments vanish $\to 0$

$$\left[\text{Now: } \sum w_i c_{i,\alpha} c_{i,\beta} c_{i,\gamma} c_{i,\sigma} = c_s^4 \left(\delta_{\alpha\beta}\delta_{\gamma\sigma} + \delta_{\alpha\gamma}\delta_{\beta\sigma} + \delta_{\alpha\gamma}\delta_{\beta\gamma}\right)\right]$$

$$= c_s^2 \begin{cases} 3\partial_1^{(1)}\partial_1^{(1)}(\rho u_1) + 2\partial_1^{(1)}\partial_2^{(1)}(\rho u_2) + \partial_2^{(1)}\partial_2^{(1)}(\rho u_1), & \alpha = 1 \\ \partial_1^{(1)}\partial_1^{(1)}\partial(\rho u_2) + 2\partial_1^{(1)}\partial_1^{(1)}(\rho u_1) + 3\partial_1^{(1)}\partial_2^{(1)}(\rho u_2), & \alpha = 2 \end{cases}$$

$$= c_s^2\left(\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + 2\partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta)\right)$$

Note: mass eqn: $\partial_\beta^{(1)} c_s^2 = c_s^2 \partial_t^{(1)} \rho = c_s^2 \partial_\beta^{(1)}(\rho u_\beta + O(\varepsilon))$

$\cancel{\partial_t(\rho u_\alpha)}$

$$\partial_t^{(2)}(\rho u_\alpha) - \Delta t\left(\frac{1}{2}-\frac{1}{\omega}\right)c_s^2 \partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta) + \Delta t\left(\frac{1}{2}-\frac{1}{\omega}\right)c_s^2\left(\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + 2\partial_\alpha^{(1)}\partial_\beta^{(1)}(\rho u_\beta)\right)$$

$$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(\frac{1}{2}-\frac{1}{\omega}\right)c_s^2\left(\partial_\beta^{(1)}\partial_\beta^{(1)}(\rho u_\alpha) + \overset{3}{\partial_\alpha^{(1)}}\underbrace{\partial_\beta^{(1)}(\rho u_\beta)}_{\nabla\cdot u_\beta}\right)$$

$$\varepsilon\partial_t^{(1)} + \varepsilon^2\partial_t^{(2)} = \partial_t$$

$$\Rightarrow \partial_t \rho + \partial_\beta(\rho u_\beta) = 0$$

use $\omega$ to tune viscosity

$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) + \partial_\alpha p = \underbrace{\Delta t\left(\frac{1}{\omega}-\frac{1}{2}\right)}_{\nu} c_s^2 \underbrace{\left(\partial_\beta\partial_\beta(\rho u_\alpha) + \partial_\alpha\partial_\beta(\rho u_\beta)\right)}_{\to \partial_\beta\partial_\beta(\rho u_\alpha)}$$

$u_\alpha \to 0$

$\rho = \text{const.}$

In vector form, this is $\nabla^2 \underline{u}$

## Numerics of LBM

- (*) Setup of LBM simulations.
- (*) Boundary conditions
- (*) Stability.

(1) Setup of LBM sim.

$0 < w < 2$ tuning viscosity — can't really go to zero in LBM, causes instability!

**LBM:** $f_i(\underline{r}+\underline{c}_i, t+1) = f_i(\underline{r},t) + w\left(f_i^{(eq)}{}_*(\underline{r},t) - f_i(\underline{r},t)\right); \; i = 0, \ldots, 8$

two cases:

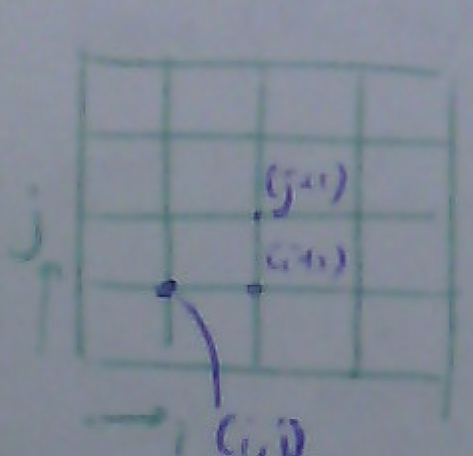
- (*) Time-dependent
- (*) Steady case

} treated the same

↳ $t = 0, 1, 2 \ldots$ until $\|u_{n+1} - u_n\| < \varepsilon$

Steady: $f_i(\underline{r}+\underline{c}_i) = f_i(\underline{r}) + w\left(f_i^{(eq)}(\underline{r}) - f_i(\underline{r})\right)$

**Recall:** grid topology




save $f_i^{(eq)}, f_i$ as

$f(k, \underbrace{i,j}_{\text{location}})$ $\quad k = 0, \ldots, 8$ $\quad i,j = 0, \ldots, N$

$\rho(i,j)$ etc.

$\underline{u} = (u,v)$ ; $u(i,j)$, $v(i,j)$

### Code outline

initial conditions

$(\rho_0, \underline{u}_0, w)$ — set such that it can recover viscosity of our system

$f_i^{(eq)}(\rho_0, u_0) \longrightarrow f_* = f^{(eq)}$

do $n = 0, 1, 2, 3, \ldots$

local computations:

- $(\rho, \underline{u})$ = macro var $(f)$ $\quad \rho = \sum f_i$, $\quad \underline{u} = \frac{1}{\rho}\sum c_i f_i$
- $f^{(eq)}$ = compute Eq $(\rho, \underline{u})$ $\quad f_i^{(eq)} = \rho w_i \{\ldots\}$
- $f \leftarrow$ collision $(f, f^{(eq)})$ $\quad f \leftarrow f + w(f^{(eq)} - f)$ ← apply source term
- $f \leftarrow$ apply b.c. $(f)$

global: $f \leftarrow$ streaming $(f)$ $\quad f_i(\underline{r}+\underline{c}_i, t+1) = f_i(\underline{r}, t)$ — collision term already added

$= \partial_t^{(2)}(\rho u_\alpha) + \Delta t\left(\frac{1}{\omega} - \frac{1}{2}\right)\partial_t^{(1)}\partial_\beta^{(1)} P_{\alpha\beta} + \Delta t\left(\frac{1}{\omega} - \frac{1}{2}\right)\partial_t^{(1)}\partial_\alpha^{(1)} \ldots$

## Setup of LBM Simulation

**given** — dimensional variable.

$\rho_{ref}^*,\ u_{ref}^*,\ \nu^*,\ L$

$\nu^*$: kinematic viscosity

$L$: characteristic length scale.

**Recall:**

$$f^{(eq)} \propto e^{\frac{-(u-c)^2}{2\boxed{RT}\,(c_s^*)^2}}$$

**Pick:** Reference Mach number

$$\text{e.g. } M = 0.01 \Rightarrow (c_s^*)^* = \frac{u_{ref}}{M}$$

$$c_0^* = \sqrt{3}\, c_s^* \quad \text{(chapter 10?)}$$

$$\Delta x^* = \frac{L}{N}$$

$$\text{since } \Delta x^* = c_0^* \Delta t^*$$

$$\Rightarrow \Delta t^* = \frac{\Delta x^*}{c_0^*}$$

$$t = \frac{t^*}{\Delta t^*} \quad (\Rightarrow \Delta t^* = 1)$$

Non-dimensionalize:

$$c_\alpha = \frac{c_\alpha^*}{c_0^*} \qquad u_\alpha = \frac{u_\alpha^*}{c_0^*} \qquad c_s^* = \frac{c_s^*}{c_0^*} \qquad \rho = \frac{\rho^*}{\rho_{ref}^*} \qquad f = \frac{f^*}{\rho_{ref}^*}$$

non-dimensionalize anyway,

$$\frac{(f_i^{(eq)})^*}{\rho_{ref}^*} = \frac{\rho^*}{\rho_{ref}^*} w_i \left\{1 + \frac{c_i^* u^*}{(c_s^*)^2} + \frac{1}{2}\frac{(c_i^* \cdot u^*)}{(c_s^*)^4} - \frac{1}{2}\frac{(u^*)^2}{(c_s^*)^2}\right\} \quad ; \quad \frac{(c_i^*)\, u^*}{(c_s^*)^2} = \frac{c_i \cdot u}{c_s^2}$$

$\rho$

$$\Rightarrow \rho w_i \{1 \ldots \quad \text{drop the } * \}$$

$$\text{if } \nu = \frac{\nu^*}{(c_0^*)^2 \Delta t^*} \qquad \text{from world, } \nu = \Delta t\left(\frac{1}{\omega} - \frac{1}{2}\right) c_s^2$$

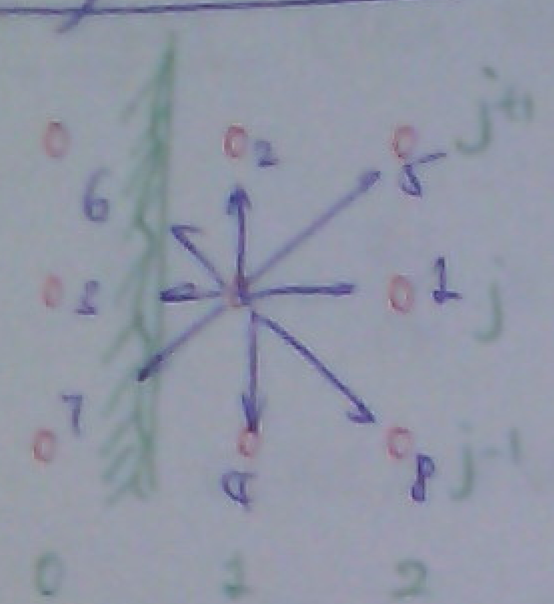
$$\Rightarrow \frac{\nu}{\Delta t c_s^2} = \frac{1}{\omega} - \frac{1}{2}$$

$$\Rightarrow \boxed{\omega = \frac{1}{\frac{\nu}{\Delta t c_s^2} + \frac{1}{2}}}$$

Note:

$$\frac{\nu}{\underbrace{\Delta t}_{=1} c_s^2} = \frac{\nu}{c_s^2} = \frac{\nu^*}{(c_0^*)^2 \Delta t^*}\frac{(c_0^*)^2}{(c_s^*)^2}$$

## Boundary Conditions




assumption,
after collision step

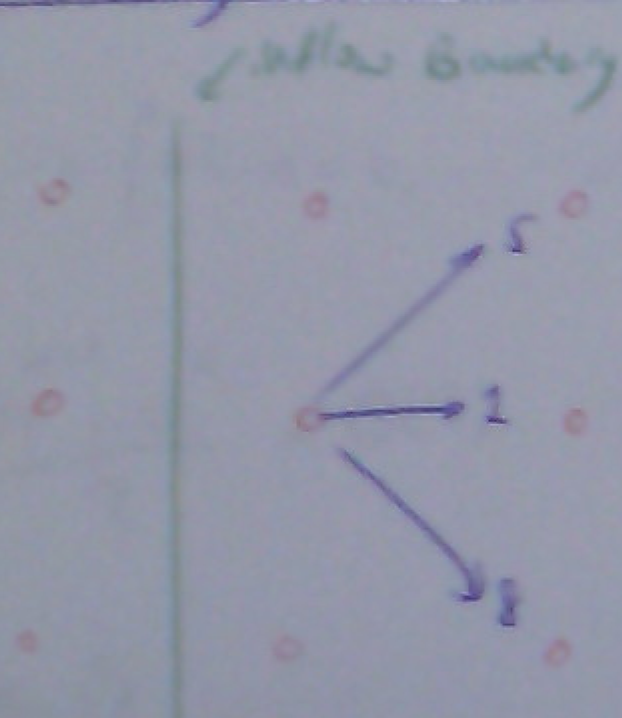
bounce back, with ghost cells

$$f_{7,0,j+1} = f_{6,1,j}$$

$$f_{1,0,j} = f_{3,1,j}$$

$$f_{5,0,j-1} = f_{7,1,j}$$

## Flux Boundary Conditions




Have $(u_0, v_0)$ at inflow

want: $\rho$, $f_1$, $f_5$, $f_8$

Have: moment relations

$$\left.\begin{aligned} \underline{u} &= \frac{1}{\rho}\sum c_i f_i \\ \rho &= \sum f_i \end{aligned}\right\} \text{three relations.}$$

2 from velocity

extra equation:

$$f_1 - f_1^{(eq)} = f_3 - f_3^{(eq)}$$

$$\Rightarrow f_1 = f_3 - \left(f_3^{(eq)} - f_1^{(eq)}\right)$$

$$\Rightarrow f_1 = f_3 + \frac{2}{3}\rho u_0$$

$$\rho = \frac{f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)}{1 - u_0}$$

$$\Rightarrow f_5 = f_7 - \frac{1}{2}(f_2 - f_4) + \frac{1}{6}\rho u_0$$

$$\Rightarrow f_8 = f_6 - \frac{1}{2}(f_4 - f_2) + \frac{1}{6}\rho u_0$$

## Stability Analysis

**Setup:**
- Assume infinite lattice
- $\rho_0, u_0$ be uniform at $t=0$.

  i.e. $\rho(\underline{r},0) =: \rho_0$, $\underline{u}(\underline{r},0) =: \underline{u}_0$ $\rightarrow f_i^{(eq)}(\underline{r},0) =: f_{i,0}^{(eq)} = \text{const.}$
- Assume $f_i(\underline{x},0)$ is uniform @ $t=0$ (e.g. $f_i = f_i^{(eq)}$)

  i.e. $f_i(\underline{x},0) = f_{i,0} = \text{const.}$ $\left(\sum f_i = \rho_0 \quad \sum c_i f_i = \rho_0 \underline{u}_0\right)$

$\boxed{\text{Consider LBM @ } t=0}$

$$f(\underline{r}+\underline{c},1) = f_i(\underline{r},0) + \omega\left(f_{i,0}^{(eq)} - f_{i,0}\right) \qquad (1)$$

dropped.

$f(\underline{r}+\underline{c},1) =: f_{i,1}$

since from beginning every node is constant in value. no matter where you go, $\underline{r}+\underline{c}$ or $\underline{r}$, the values are the same, hence the $\underline{c}$ in LHS can be dropped

$$\Rightarrow f_{i,1} = (1-\omega) f_{i,0} + \omega f_{i,0}^{(eq)} \quad (*)$$

$$\Rightarrow \sum f_{i,1} = (1-\omega) \underbrace{\sum f_{i,0}}_{\rho} + \omega \underbrace{\sum f_{i,0}^{(eq)}}_{\rho}$$

similarly for $\rho_0 \underline{u}_0$

even if this is known to be $\rho$ for both terms $f_{i,1}$ is not guaranteed to be constant.

Subtract $f_{i,0}^{(eq)}$ from (1)

$$\Rightarrow \tilde{f}_{i,1} = f_{i,1} - f_{i,0}^{(eq)} = (1-\omega) f_{i,0} + (\omega - 1) f_{i,0}^{(eq)}$$
$$= (1-\omega)\underbrace{\left(f_{i,0} - f_{i,0}^{(eq)}\right)}_{\tilde{f}_{i,0}}$$

$$\Rightarrow \tilde{f}_{i,1} = (1-\omega)\tilde{f}_{i,0}$$

$\boxed{\text{RECURSION PROOF}}$

$(*) \rightarrow f_{i,2} = (1-\omega) f_{i,1} + \omega f_{i,1}^{(eq)}$ $\quad f_{i,1}^{(eq)} = f_{i,0}^{(eq)}$ (because $\rho, u$ are same) $\rightarrow$ subtract $f_{i,0}^{(eq)} \Rightarrow \tilde{f}_{i,2} = (1-\omega)\tilde{f}_{i,1} = (1-\omega)^2 \tilde{f}_{i,0}$

$$\Rightarrow \tilde{f}_{i,k} = (1-\omega)^k \tilde{f}_{i,0}$$

Need $|1-\omega| \leq 1$

$\Rightarrow 0 \leq \omega \leq 2$

LBM

(1) 3rd Feb 2017

(i) linear Stability Analysis.

(ii) H - Theorem

Fourier Analysis (Von Neumann test)

Example:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \qquad x \in [0, 2\pi),\ a > 0$$

$$u(x,t) = u(x+2\pi, t) \quad \forall t$$

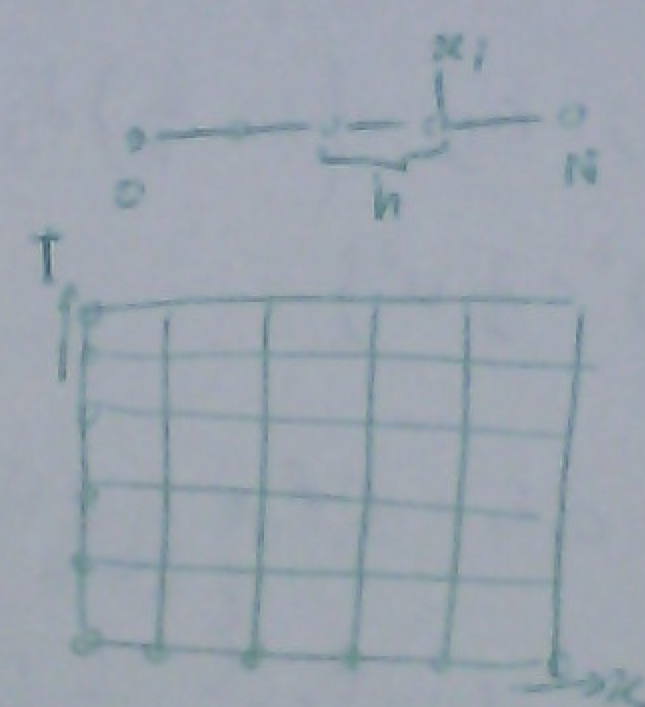
$$u(x,0) = u_0(x)$$

$$u_0(x+2\pi) = u(x)$$

Finite Difference:

$$g_h := \{ih : i = 0, \dots, N;\ hN = 2\pi\}$$

$$g_\tau := \{n\tau : n = 0, \dots, M;\ M\tau = T\}$$




$[0, 2\pi) \times [0, T]$

$$u_t^{(x_i, t^n)} = \frac{u_i^{n+1} - u_i^n}{\tau} + O(\tau)$$

$$u_i^n = u(x_i, t^n)$$

$$u_x = \frac{u_i^n - u_{i-1}^n}{h} + O(h)$$

$$\Rightarrow \frac{u_i^{n+1} - u_i^n}{\tau} + a\frac{u_i^n - u_{i-1}^n}{h} = 0 \qquad \Rightarrow u_i^{n+1} = u_i^n - \nu(u_i^n - u_{i-1}^n);\ \nu = \frac{a\tau}{h}$$

Fourier:

$$u_i^n = \sum_{k=0}^{N-1} c_k^n e^{\overset{\text{imaginary}}{i}khi} \quad \star$$

Substitute into scheme:

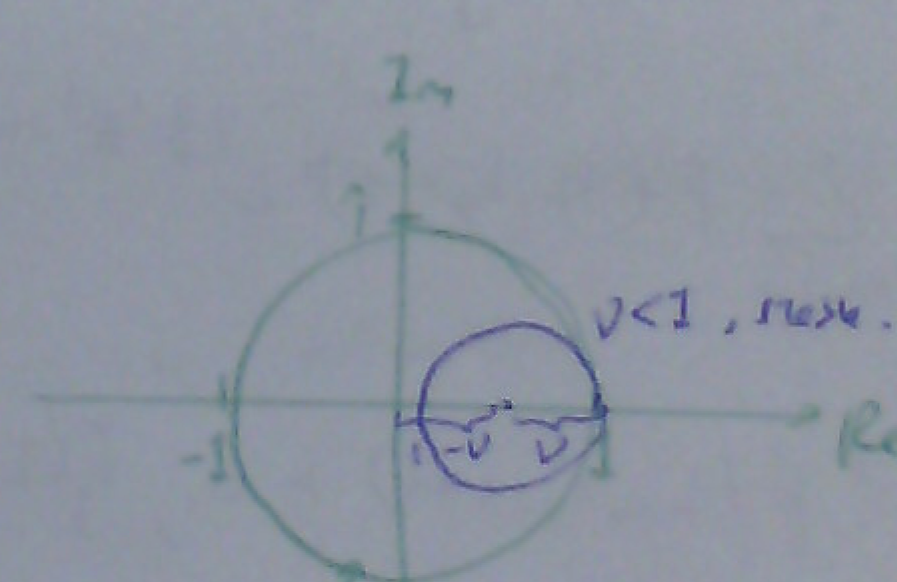
$$c_k^{n+1} e^{ikih} = c_k^n\left(e^{ikih} - \nu\left(e^{ikih} - e^{ik(i-1)h}\right)\right)$$

$$\Rightarrow \left|\frac{c_k^{n+1}}{c_k^n}\right| = \left|1 - \nu\left(1 - e^{-ikh}\right)\right| \le 1$$

bounded by 1, means

$$, e^{ix} = \cos x + i\sin x$$

$$\underbrace{1 - \nu + \underbrace{\nu \underbrace{e^{-ikh}}_{\text{gives a unit circle.}}}_{\text{unit circle with radius } \nu}}_{\text{unit circle with radius } \nu \text{ shifted to } 1-\nu \text{ away from zero.}}$$



## Application to LBM

$$f_i(x+c_i, t+1) = \underbrace{f_i(x,t) + \frac{1}{\tau}\left(f_i^{(eq)}(x,t) - f_i(x,t)\right)}_{g_i}$$

"nonlinear" comes from $f_i^{(eq)}$

$f_i^{(eq)} = f_i^{(eq)}(\rho, \underline{m})$ ; $\rho = \sum_i f_i$, $\underline{m} = \sum_i c_i f_i$ ($\rho\underline{u}$)

$f_i^{(eq)} \equiv f_i^{(eq)}(\rho(\underline{f}), \underline{m}(\underline{f}))$ ; $\underline{f} = (f_0, \dots, f_8)^T$

Apply von Neumann $\Rightarrow$ linearize!

$f_i = \overline{f_i^{(eq)}} + f_i'$

const + f(x)

$$\overline{f^{(eq)}} + \frac{1}{\tau}\underbrace{\left(f_i^{(eq)}(\rho(\overline{f^{(eq)}}), \underline{m}(\overline{f^{(eq)}})) - \overline{f_i^{(eq)}}\right)}_{=0}$$

$$\overline{f_i^{(eq)}} + f_i'(x+c_i, t+1) = g_i(\overline{f^{(eq)}}) + \left.\frac{\partial g_i}{\partial f_j}\right|_{\overline{f^{(eq)}}} f_j'$$

differentiate first! then substitute with $\overline{f^{(eq)}}$

summation

$$\Rightarrow \cancel{\overline{f_i^{(eq)}}} + f_i'(x+c_i, t+1) = \cancel{\overline{f_i^{(eq)}}} + f_i' + \frac{1}{\tau}\left(\frac{\partial f_i^{(eq)}}{\partial f_j} f_j' - f_i'\right)$$

$$f_i'(x+c_i, t+1) = G_{ij} f_j'(x,t) \; ; \quad G_{ij} = \left(1 - \frac{1}{\tau}\right)\delta_{ij} + \frac{1}{\tau}\frac{\partial f_i^{(eq)}}{\partial f_j}$$

$$f_i^{(eq)} = w_i \rho \left\{1 + 3 c_i \cdot \underline{u} + \frac{9}{2}(c_i \cdot \underline{u})^2 - \frac{3}{2}u^2\right\}$$

$$\left[\rho = \sum f_i \qquad \rho\underline{u} \equiv \underline{m} = \sum c_i f_i = c_0 f_0 + c_1 f_1 + \dots + c_8 f_8\right]$$

$$\Rightarrow f_i^{(eq)} = w_i\left\{\rho + 3 c_i \cdot \underline{m} + \frac{9}{2}\cdot\frac{1}{\rho} c_i \cdot (\underbrace{\rho\underline{u}}_{\underline{m}})^2 - \frac{3}{2}\cdot\frac{1}{\rho}(\underbrace{\rho\underline{u}}_{\underline{m}})^2\right.$$

$\rho = \sum f_i$

$$\frac{\partial f_i^{(eq)}}{\partial f_j} = w_i\left\{1 + 3 c_i \cdot c_j + \frac{9}{2}\left(-\frac{1}{\rho^2}\right)(c_i \cdot \rho\underline{u})^2 + \frac{9}{2}\frac{1}{\rho} 2(c_i \cdot \cancel{c_j}(\rho\underline{u}))(c_i \cdot c_j) + \frac{3}{2}\left(-\frac{1}{\rho^2}\right)|\rho\underline{u}|^2\right.$$
$$\left. + \frac{3}{2}\cdot\frac{1}{\rho} 2\rho\underline{u}\cdot c_j\right\}$$

now, in the ..., u is independent of $\rho$.

$$= w_i\left\{1 + 3 c_i \cdot c_j + \frac{9}{2}\left(2(c_i \cdot c_j)(c_i \cdot \underline{u}) - (c_i \cdot \underline{u})^2\right) + \frac{3}{2}\left(2 c_j \cdot \underline{u} - |\underline{u}|^2\right)\right.$$

$$f_i'(x,t) = \sum_{k_x, k_y} F(k_x, k_y, t)\, e^{\hat{\imath}\underline{k}\cdot\underline{x}} \quad ; \; \underline{k} = [k_x \; k_y]^T$$

Substitute!

$$e^{\hat{\imath}\underline{k}\cdot(\underline{x}+c_i)} F_i(k_x, k_y, t+1) = G_{ij} F_j(k_x, k_y, t)\, e^{\hat{\imath}\underline{k}\cdot\underline{x}}$$

$$\Rightarrow F_i(k_x, k_y, t+1) = \underbrace{G_{ij}\, e^{-\hat{\imath}\underline{k}\cdot c_i}}_{\Gamma_{ij}} F_j(k_x, k_y, t)$$

Read stability analysis on LBM (posted by Prof. May)

$$f_i(t+s) - f^{(0)}(t) = f_i(t) - f_i^{(0)}(t) + s\omega\left(f_i^{(0)}(t) - f_i(t)\right) = (-1+s\omega)\left(f_i^{(0)}(t) - f_i(t)\right)$$

$$\Rightarrow f_i^{(0)} - f_i = \frac{f_i(t+s) - f_i^{(0)}(t)}{s\omega - 1}$$

$$= \frac{f_i^{(0)}(t) - f_i(t+s)}{1 - s\omega}$$

(*) $= \tilde{h}(t+1) - \tilde{h}(t)$

$$= \underbrace{\int_0^1 \underbrace{\left(h_i'(f(t+s)) - h_i'(f^{(0)}(t))\right)}_{\Delta h_i'} \underbrace{\frac{\omega}{1-s\omega}}_{\geq 0} \underbrace{\left(f_i^{(0)}(t) - f_i(t+s)\right)}_{-\Delta f_i} ds}_{\leq 0}$$

$h_i$ convex

$$\Rightarrow \frac{\Delta h_i'}{\Delta f} \geq 0 \quad \Big| \cdot \underbrace{(\Delta f)^2}_{\geq 0}$$

$$\Leftrightarrow \Delta f \cdot \Delta h_i' \geq 0$$

$$\Leftrightarrow -\Delta f \, \Delta h_i' \leq 0$$

$$(h_i')^{-1}(x) = a + bx + cx^2 = f_i^{(0)} \quad ; \quad x = \underset{a = a(\rho, u)}{a} + \underset{b(\rho, u)}{\underline{b}} \cdot s_i \qquad \sum f_i^{(0)} = \rho \qquad \sum f_i^{(0)} = \rho \underline{u}$$

theoretically its possible to have entropic scheme (stable out of the box), but not at the moment!

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**Exam:**

→ Continuum mechanics:

→ Conservation laws.
- constitutive laws } where does it come from?
- equations of states
  empirical laws

→ Kinetic theory
- collision models. — for equilibrium fill collision terms
- Maxwell - Boltzmann ← maxwellian is sufficient condition
  - ↳ H - theorem
- Boltzmann Eq. ← should be able to write it down
  } connected by moments. should know how.
- Conservation laws
- local thermodynamic equilibrium
  - ↳ Euler equations.
- BGK eq should know. BGK only has 1 free coefficient, τ! causes fixed heat conduction coeff. } related to Prandtl number.
- Chapman enskog. should know the assumptions, steps needed to derive NS. } leads to NS*
  - ↳ are there difference with NS.

## LBM

② 3rd Feb 2017

**Recall:** Boltzmann eq.: $\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = J(f,f)$

H-function $\quad H := \int f \ln f \, \cancel{d} \, d\underline{c}$

H-theorem :

$$\frac{dH}{dt} \leq 0$$

maxwell-boltzmann dist.

$$\frac{dH}{dt} = 0 \iff f \equiv f^{(MB)}$$

$$f^{(MB)} = \text{argmin} \{ H(f) : n = \int_{\mathbb{R}^3} f \, d\underline{c}$$

$= (\rho, u, T)$

$$n\underline{u} = \int_{\mathbb{R}^3} \underline{c} f \, d\underline{c}$$

number density

$$\frac{3}{2} n k_B T = \int_{\mathbb{R}} (\underline{c} - \underline{u})^2 f \, d\underline{c} \}$$

**LBM:**

$$f_i(\underline{r} + \underline{c}_i, t+1) = f_i(\underline{r}, t) + \omega \left( f_i^{(eq)}(\underline{r}, t) - f_i(\underline{r}, t) \right)$$

$\omega = \frac{1}{\tau}$

convex function

$$H = \sum_{i=0}^{N_L^d} h_i(f_i(\underline{r}, t)) = \sum \tilde{h}_i(\underline{r}, t) \quad ; \tilde{h}_i = h_i \cdot f_i$$

Look for

$$f_i^{(e)} = \text{argmin} \{ H(f) : \rho = \sum f_i \,;\, \rho u = \sum c_i f_i \}$$

want this to be monotone. (i.e. not grow during collision process!) so that $\omega(f_i^{(e)} - f_i)$ will monotonously decrease ~~H(f)~~ $H(f)$

to solve this "look for $f_i^{(e)}$", we use lagrangian multiplier.

Only need to look for collision part, as streaming part just redistributes distributions.